AMOP reference links on following page

3.02.18 class 14.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

Discrete symmetry subgroups of O(3) using Mock-Mach principle: $D_3 \sim C_{3v}$ LAB vs BOD
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D_6 Band structure and related Global vs Local induced representations, D_4 example

U(12)-Supersymmetry

AMOP reference links *(Updated list given on 2nd page of each class presentation)*

Web Resources - front page
UAF Physics UTube channel

Quantum Theory for the Computer Age
Principles of Symmetry, Dynamics, and Spectroscopy
Classical Mechanics with a Bang!
Modern Physics and its Classical Foundations

2014 AMOP
2017 Group Theory for QM
2018 AMOP

Frame Transformation Relations And Multipole Transitions In Symmetric Polyatomic Molecules - RMP-1978
Rotational energy surfaces and high- J eigenvalue structure of polyatomic molecules - Harter - Patterson - 1984
Galloping waves and their relativistic properties - ajp-1985-Harter
Asymptotic eigensolutions of fourth and sixth rank octahedral tensor operators - Harter-Patterson-JMP-1979
Nuclear spin weights and gas phase spectral structure of 12C60 and 13C60 buckminsterfullerene -Harter-Reimer-Cpl-1992 - (Alt1, Alt2 Erratum)

Theory of hyperfine and superfine levels in symmetric polyatomic molecules.

I) Trigonal and tetrahedral molecules: Elementary spin-1/2 cases in vibronic ground states - PRA-1979-Harter-Patterson (Alt scan)
II) Elementary cases in octahedral hexafluoride molecules - Harter-PRA-1981 (Alt scan)

Rotation-vibration scalar coupling zeta coefficients and spectroscopic band shapes of buckminsterfullerene - Weeks-Harter-CPL-1991 (Alt scan)
Fullerene symmetry reduction and rotational level fine structure/ the Buckyball isotopomer 12C 13C59 - jcp-Reimer-Harter-1997 (HiRez)
Molecular Eigensolution Symmetry Analysis and Fine Structure - IJMS-harter-mitchell-2013

Rotation–vibration spectra of icosahedral molecules.

I) Icosahedral symmetry analysis and fine structure - harter-weeks-jcp-1989
II) Icosahedral symmetry, vibrational eigenfrequencies, and normal modes of buckminsterfullerene - weeks-harter-jcp-1989
III) Half-integral angular momentum - harter-reimer-jcp-1991

QTCA Unit 10 Ch 30 - 2013
AMOP Ch 32 Molecular Symmetry and Dynamics - 2019
AMOP Ch 0 Space-Time Symmetry - 2019

RESONANCE AND REVIVALS

I) QUANTUM ROTOR AND INFINITE-WELL DYNAMICS - ISMSLi2012 (Talk) OSU knowledge Bank
II) Comparing Half-integer Spin and Integer Spin - Alva-ISMS-Ohio2013-R777 (Talks)
III) Quantum Resonant Beats and Revivals in the Morse Oscillators and Rotors - (2013-Li-Diss)

Rovibrational Spectral Fine Structure Of Icosahedral Molecules - Cpl 1986 (Alt Scan)
Gas Phase Level Structure of C60 Buckyball and Derivatives Exhibiting Broken Icosahedral Symmetry - reimer-diss-1996
Resonance and Revivals in Quantum Rotors - Comparing Half-integer Spin and Integer Spin - Alva-ISMS-Ohio2013-R777 (Talk)
Quantum Revivals of Morse Oscillators and Farey-Ford Geometry - Li-Harter-cpl-2013
Wave Node Dynamics and Revival Symmetry in Quantum Rotors - harter - jms - 2001

**In development - a web based A.M.O.P. oriented reference page, with thumbnail/previews, greater control over the information display, and eventually full on* Apache-SOLR *Index and search for* nuanced, whole-site content/metadata level *searching. This bad boy will be a sure force multiplier.*

AMOP reference links on page 2

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D_3 Hamiltonian *local-* $\mathbf{H}$ *matrices in* $|\mathbf{P}^{(\mu)}\rangle$*-basis*

$\mathbf{H}$ *matrix in* $|\mathbf{g}\rangle$*-basis:*

$$(\mathbf{H})_G = \sum_{g=1}^{^oG} r_g \bar{\mathbf{g}} = \begin{pmatrix} r_0 & r_2 & r_1 & i_1 & i_2 & i_3 \\ r_1 & r_0 & r_1 & i_3 & i_1 & i_2 \\ r_2 & r_1 & r_0 & i_2 & i_3 & i_1 \\ i_i & i_3 & i_2 & r_0 & r_1 & r_2 \\ i_2 & i_1 & i_3 & r_2 & r_0 & r_1 \\ i_3 & i_2 & i_1 & r_1 & r_2 & r_0 \end{pmatrix}$$

$\mathbf{H}$ *matrix in* $|\mathbf{P}^{(\mu)}\rangle$*-basis:*

$$(\mathbf{H})_P = \bar{T}(\mathbf{H})_G \bar{T}^\dagger = \begin{array}{c} \begin{array}{cccccc} |\mathbf{P}^{A_1}_{xx}\rangle & |\mathbf{P}^{A_2}_{yy}\rangle & |\mathbf{P}^{E_1}_{xx}\rangle & |\mathbf{P}^{E_1}_{xy}\rangle & |\mathbf{P}^{E_1}_{yx}\rangle & |\mathbf{P}^{E_1}_{yy}\rangle \end{array} \\ \left(\begin{array}{c|c|cc|cc} H^{A_1} & \cdot & \cdot & \cdot & \cdot & \cdot \\ \hline \cdot & H^{A_2} & \cdot & \cdot & \cdot & \cdot \\ \hline \cdot & \cdot & H^{E_1}_{xx} & H^{E_1}_{xy} & \cdot & \cdot \\ \cdot & \cdot & H^{E_1}_{yx} & H^{E_1}_{yy} & \cdot & \cdot \\ \hline \cdot & \cdot & \cdot & \cdot & H^{E_1}_{xx} & H^{E_1}_{xy} \\ \cdot & \cdot & \cdot & \cdot & H^{E_1}_{yx} & H^{E_1}_{yy} \end{array}\right) \end{array}$$

$$H^{\alpha}_{ab} = \langle \mathbf{P}^{\mu}_{ma}|\mathbf{H}|\mathbf{P}^{\mu}_{nb}\rangle = \underset{(norm)^2}{\underline{\langle \mathbf{1}|\mathbf{P}^{\mu}_{am}\mathbf{H}\mathbf{P}^{\mu}_{nb}|\mathbf{1}\rangle}} = \langle \mathbf{1}|\mathbf{H}\mathbf{P}^{\mu}_{am}\underset{(norm)^2}{\underline{\mathbf{P}^{\mu}_{nb}|\mathbf{1}\rangle}} = \delta_{mn}\underset{(norm)^2}{\underline{\langle \mathbf{1}|\mathbf{H}\,\mathbf{P}^{\mu}_{ab}|\mathbf{1}\rangle}} = \sum_{g=1}^{^\circ G}\langle \mathbf{1}|\mathbf{H}|\mathbf{g}\rangle D^{\alpha *}_{ab}(g) = \sum_{g=1}^{^\circ G} r_g D^{\alpha *}_{ab}(g)$$

$$H^{A_1} = r_0 D^{A_1 *}(1) + r_1 D^{A_1 *}(r^1) + r_1^* D^{A_1 *}(r^2) + i_1 D^{A_1 *}(i_1) + i_2 D^{A_1 *}(i_2) + i_3 D^{A_1 *}(i_3) = r_0 + r_1 + r_1^* + i_1 + i_2 + i_3 \quad = r_0 + 2r_1 + 2i_{12} + i_3$$

$$H^{A_2} = r_0 D^{A_2 *}(1) + r_1 D^{A_2 *}(r^1) + r_1^* D^{A_2 *}(r^2) + i_1 D^{A_2 *}(i_1) + i_2 D^{A_2 *}(i_2) + i_3 D^{A_2 *}(i_3) = r_0 + r_1 + r_1^* - i_1 - i_2 - i_3 \quad = r_0 + 2r_1 - 2i_{12} - i_3$$

$$H^{E_1}_{xx} = r_0 D^{E*}_{xx}(1) + r_1 D^{E*}_{xx}(r^1) + r_1^* D^{E*}_{xx}(r^2) + i_1 D^{E*}_{xx}(i_1) + i_2 D^{E*}_{xx}(i_2) + i_3 D^{E*}_{xx}(i_3) = (2r_0 - r_1 - r_1^* - i_1 - i_2 + 2i_3)/2 \quad = r_0 - r_1 - i_{12} + i_3$$

$$H^{E_1}_{xy} = r_0 D^{E*}_{xy}(1) + r_1 D^{E*}_{xy}(r^1) + r_1^* D^{E*}_{xy}(r^2) + i_1 D^{E*}_{xy}(i_1) + i_2 D^{E*}_{xy}(i_2) + i_3 D^{E*}_{xy}(i_3) = \sqrt{3}(-r_1 + r_1^* - i_1 + i_2)/2 = H^{E*}_{yx} \quad = 0$$

$$H^{E_1}_{yy} = r_0 D^{E*}_{yy}(1) + r_1 D^{E*}_{yy}(r^1) + r_1^* D^{E*}_{yy}(r^2) + i_1 D^{E*}_{yy}(i_1) + i_2 D^{E*}_{yy}(i_2) + i_3 D^{E*}_{yy}(i_3) = (2r_0 - r_1 - r_1^* + i_1 + i_2 - 2i_3)/2 \quad = r_0 - r_1 + i_{12} - i_3$$

$C_2 = \{\mathbf{1}, \mathbf{i_3}\}$
Local symmetry determines all levels and eigenvectors with just 4 real parameters

$$\begin{pmatrix} H^{E_1}_{xx} & H^{E_1}_{xy} \\ H^{E_1}_{yx} & H^{E_1}_{yy} \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 2r_0 - r_1 - r_1^* - i_1 - i_2 + 2i_3 & \sqrt{3}(-r_1 + r_1^* - i_1 + i_2) \\ \sqrt{3}(-r_1^* + r_1 - i_1 + i_2) & 2r_0 - r_1 - r_1^* + i_1 + i_2 - 2i_3 \end{pmatrix}$$

$$= \begin{pmatrix} r_0 - r_1 - i_{12} + i_3 & 0 \\ 0 & r_0 - r_1 - i_{12} - i_3 \end{pmatrix}_{For:\, r_1 = r_1^* \, and:\, i_1 = i_2}$$

Choosing local $C_2 = \{\mathbf{1}, \mathbf{i_3}\}$ *symmetry with local constraints* $r_1 = r_1^* = r_2$ *and* $i_1 = i_2$

$D_3 > C_2\,\mathbf{i}_3$ projector states

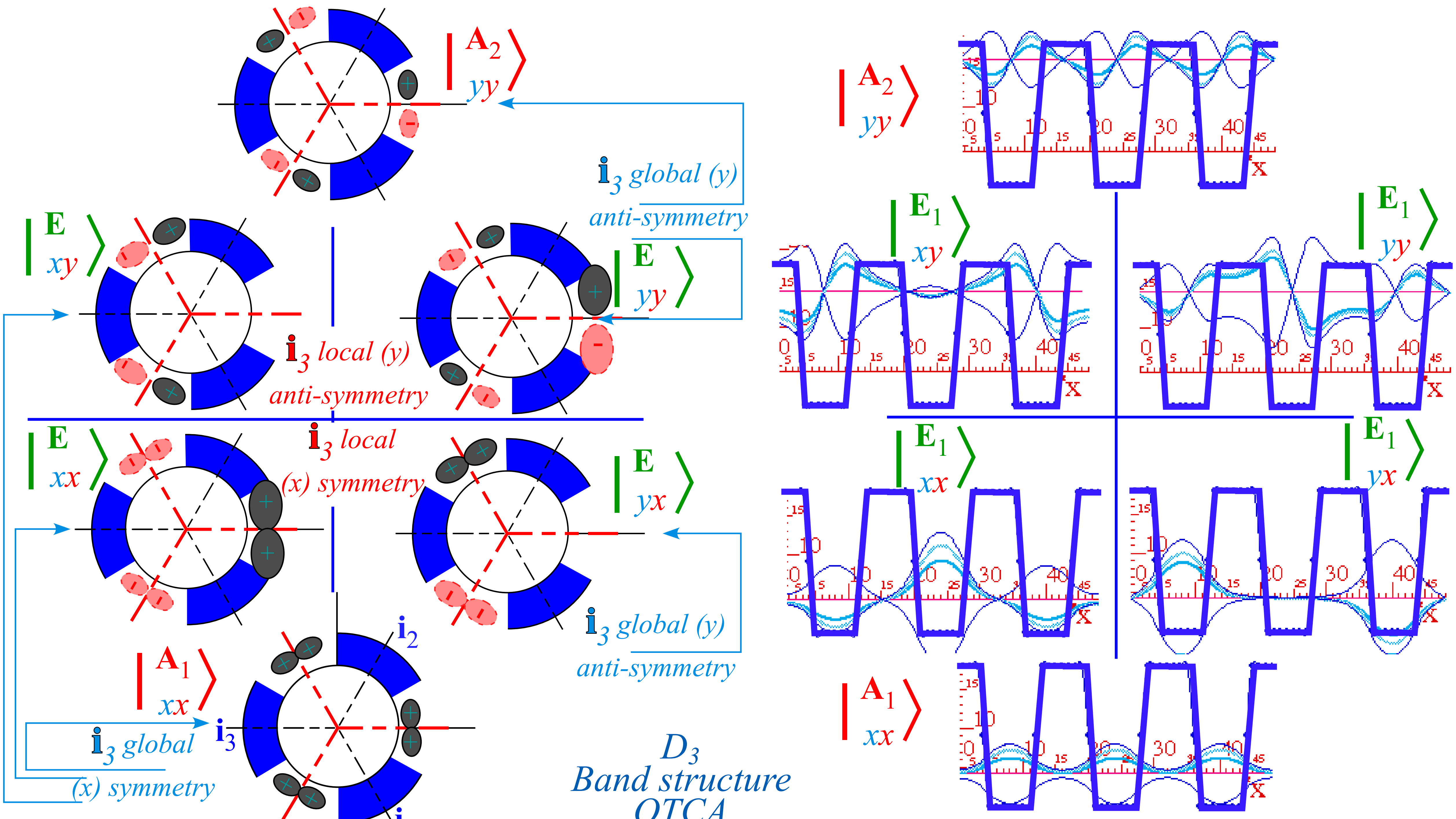
$$|^{(m)}_{eb}\rangle = \mathbf{P}^{(m)}_{eb}|1\rangle$$

Global (LAB) symmetry

$$\mathbf{i}_3|^{(m)}_{eb}\rangle = \mathbf{i}_3\mathbf{P}^{(m)}_{eb}|1\rangle = (-1)^e\,|^{(m)}\rangle$$

Local (BOD) symmetry

$$\bar{\mathbf{i}}_3|^{(m)}_{eb}\rangle = \bar{\mathbf{i}}_3\mathbf{P}^{(m)}_{eb}|1\rangle = \mathbf{P}^{(m)}_{eb}\bar{\mathbf{i}}_3|1\rangle = \mathbf{P}^{(m)}_{eb}\mathbf{i}_3^{\dagger}|1\rangle = (-1)^b\,|^{(m)}\rangle$$



D_3
Band structure
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Molecular vibrational modes vs. Hamiltonian eigenmodes

Classical equations of coupled harmonic motion are Newtonian $\mathbf{F}=\mathbf{M}\cdot\mathbf{a}$ relations of n-dimensional force vector $\mathbf{F}$, acceleration vector $\mathbf{a}$, and mass operator $\mathbf{M}=M\cdot\mathbf{1}$ for D_3-symmetry. Force $\mathbf{F}$ is a (-)derivative of potential $V(x)$ that becomes a $\mathbf{F}=-\mathbf{K}\cdot\mathbf{x}$ matrix expression.

$$-M\partial_t^2 x^a = \frac{\partial V}{\partial x^a} = \sum_b K_{ab} x^b$$

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Compare classical equation to Schrodinger's equation for quantum motion.† †

$$i\hbar\partial_t \psi^a = \sum_b H_{ab} \psi^b$$

† *Recall U(2) vs R(3) Schrodinger vs Classical analogs in Lect. 4 p14*

†*Int. Journal of Molec. Sci. (2013) page 798-804 pdf page85*

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Squared time generator $(i\hbar\partial_t=\mathbf{H})^2$ has classical form with K=H^2 and M=$\hbar^2$.

$$-\hbar^2\partial_t^2\psi^a = \sum_b K_{ab}\psi^b \text{ where: } K = H^2$$

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And, each eigen*value* set corresponds to its respective energy spectrum.

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Classical modes are eigenvectors of force-field matrix K or operator $\mathbf{K}$.

Harmonic potential $V(\mathbf{x})$ is a quadratic K-form of coordinates x_a based on six D_3-labeled axes $\hat{\mathbf{x}}^a$ or $|a\rangle$.

$$V(x) = \sum_{(k)} \frac{1}{2} \langle x|\mathbf{K}|x\rangle \quad \text{where:} \quad |x\rangle = \sum_a x_a |a\rangle \;, \quad (a,b) = (1, r^1, r^2, i_1, i_2, i_3)$$

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Each $\mathbf{K}$ component $K_{ab}=\langle a|\mathbf{K}|b\rangle$ is a sum over spring k-constants that connect axis-$\mathbf{x}^a$ to axis-$\mathbf{x}^b$ multiplied by factor $(\hat{\mathbf{k}}_a \bullet \hat{\mathbf{x}}^a)(\hat{\mathbf{k}}_b \bullet \hat{\mathbf{x}}^b)$ for projecting spring-k's end vectors $\hat{\mathbf{k}}_a$ and $\hat{\mathbf{k}}_b$ onto $\hat{\mathbf{x}}^a$ and $\hat{\mathbf{x}}^b$ at respective connections.

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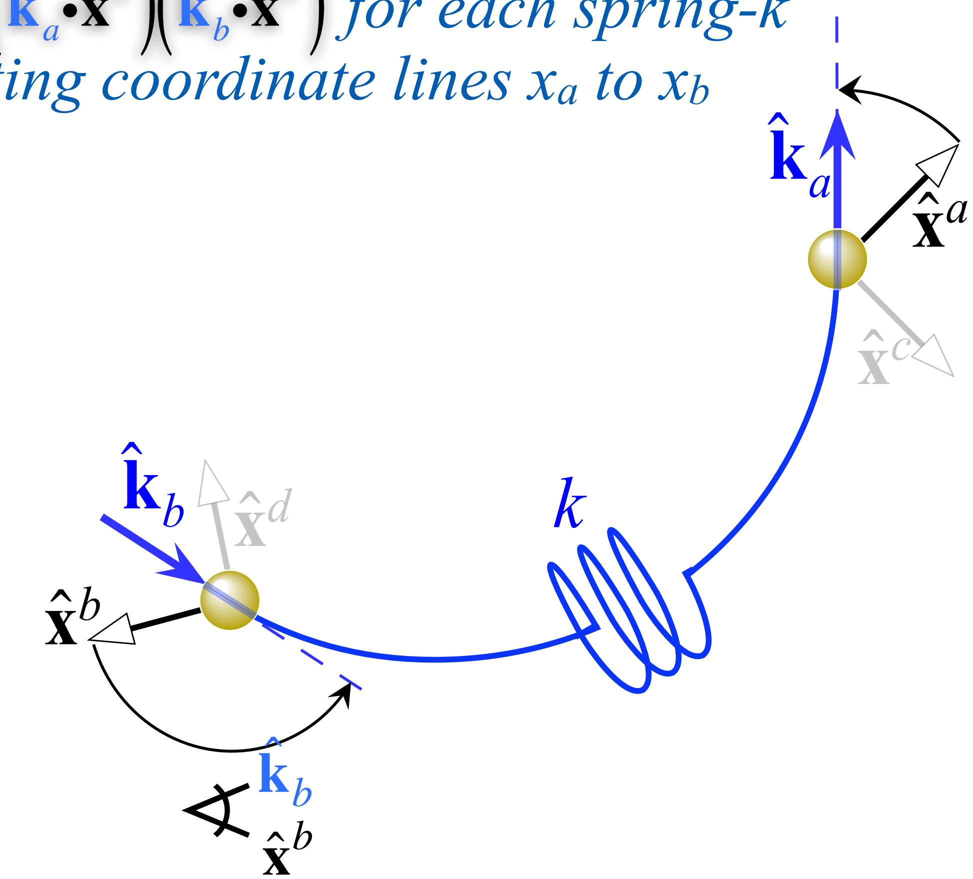
Coupling $K_{ab}=\langle a|\mathbf{K}|b\rangle$

Sum $k\cdot\left(\hat{\mathbf{k}}_a\bullet\hat{\mathbf{x}}^a\right)\left(\hat{\mathbf{k}}_b\bullet\hat{\mathbf{x}}^b\right)$ *for each spring-k connecting coordinate lines* x_a *to* x_b



Molecular K-matrix construction

Classical modes are eigenvectors of force-field matrix K or operator $\mathbf{K}$.

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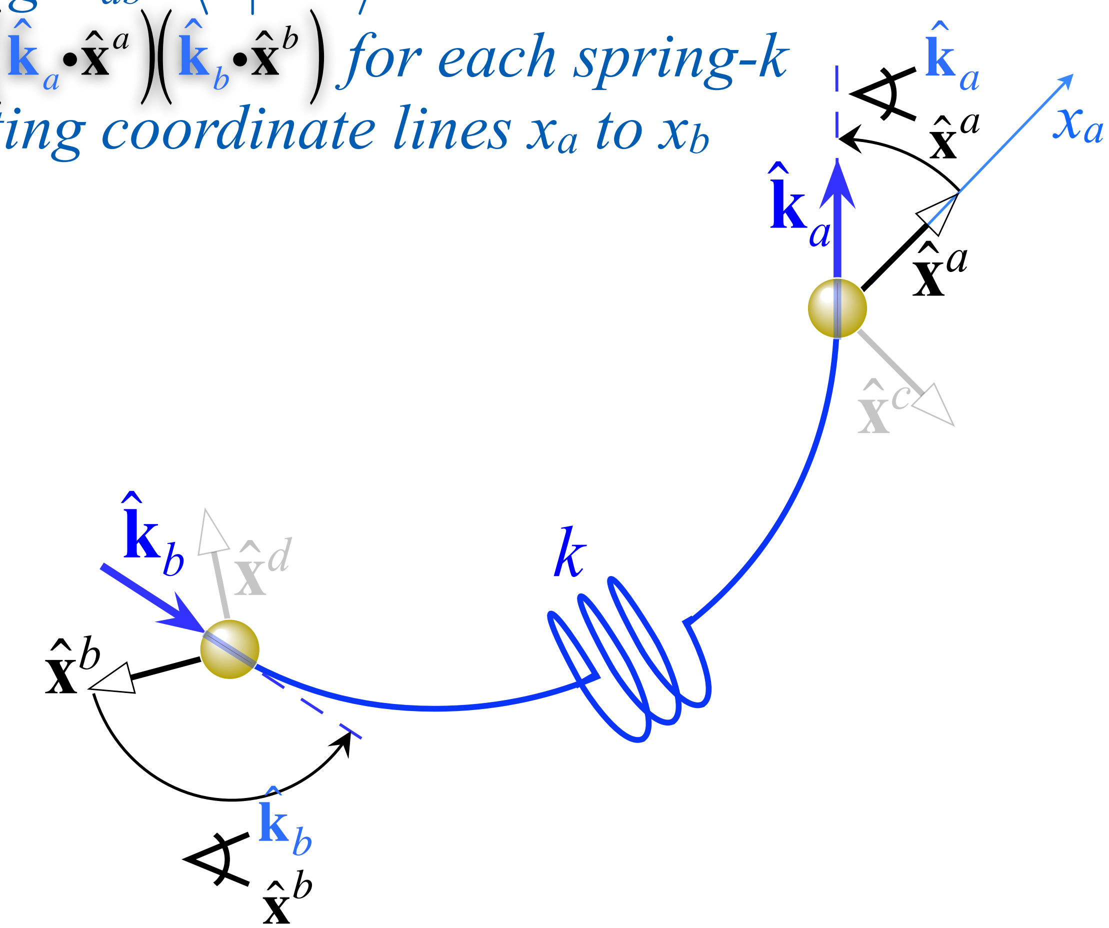
Diagonal $K_{aa}{=}\langle a|\mathbf{K}|a\rangle$
Sum $-\frac{1}{2}k\cdot(\hat{\mathbf{k}}_a{\bullet}\hat{\mathbf{x}}^a)^2$ *for each spring-k connected to coordinate line* x_a



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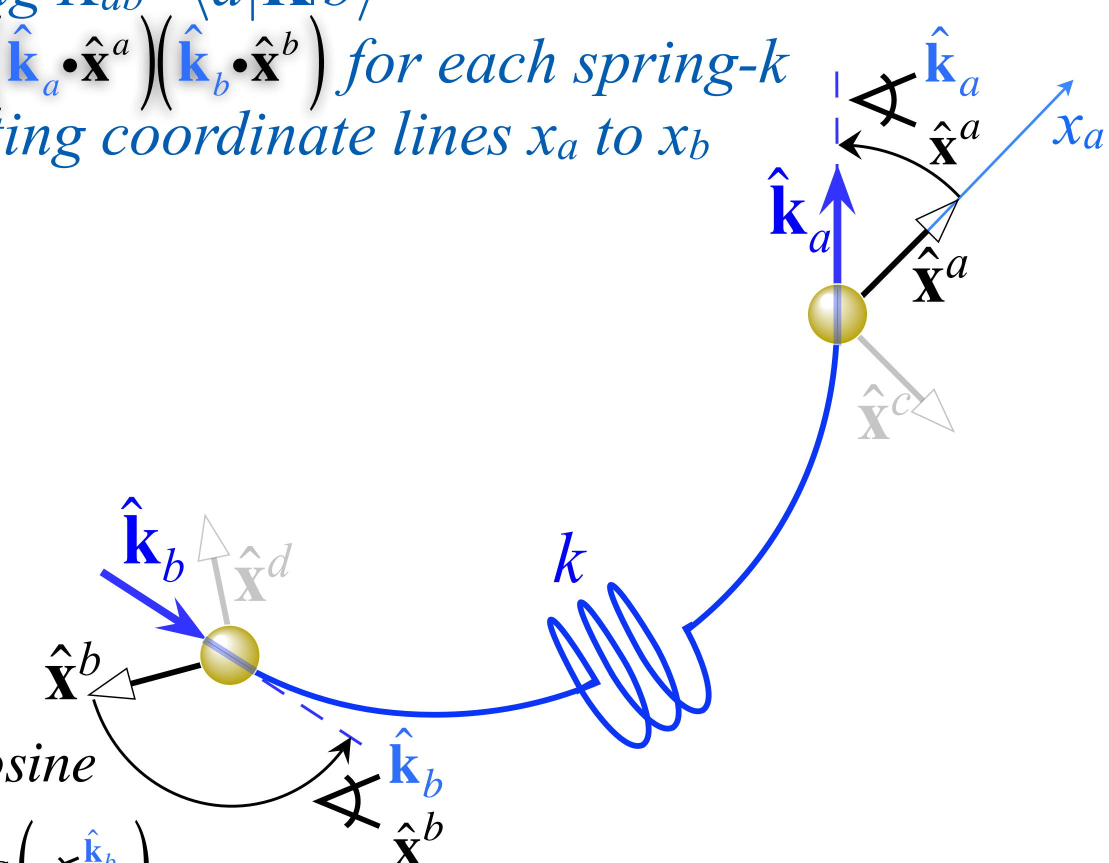

Direction cosine
$\left(\hat{\mathbf{k}}_b\bullet\hat{\mathbf{x}}^b\right) = \cos\left(\measuredangle^{\hat{\mathbf{k}}_b}_{\hat{\mathbf{x}}^b}\right)$
at b-end of k - spring

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$$V(x) = \sum_{(k)} \frac{k}{2} (\Delta \ell_k)^2 = \sum_{(k)} \frac{k}{2} \sum_{a,b} (\hat{\mathbf{k}}_a \bullet \mathbf{x}^a - \hat{\mathbf{k}}_b \bullet \mathbf{x}^b)^2$$

$$= \sum_{(k)} \frac{k}{2} \sum_a (\hat{\mathbf{k}}_a \bullet \hat{\mathbf{x}}^a)^2 x_a^2 - \sum_{(k)} k \sum_{a \neq b} (\hat{\mathbf{k}}_a \bullet \hat{\mathbf{x}}^a)(\hat{\mathbf{k}}_b \bullet \hat{\mathbf{x}}^b) x_a x_b$$

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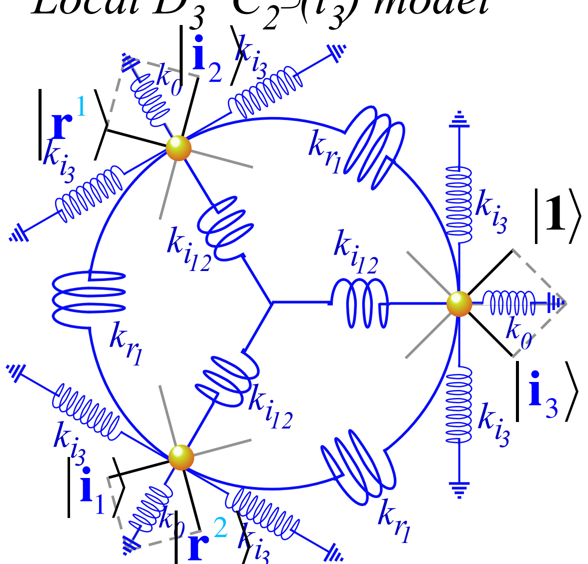
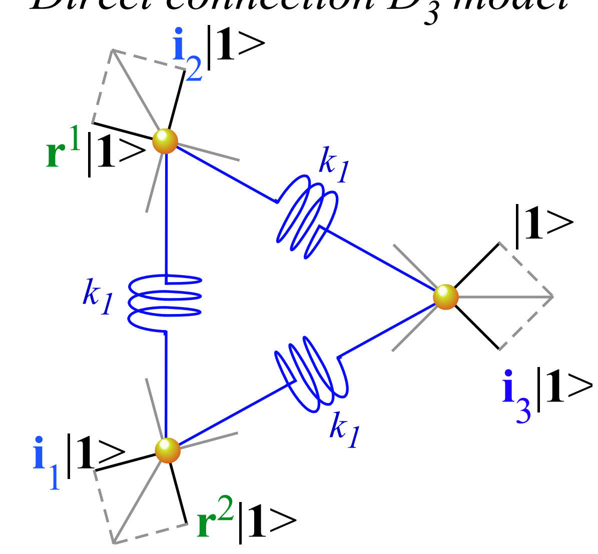
Local D_3 $C_2 \supset (i_3)$ model



Direct connection D_3 model



AMOP reference links on page 2

2.26.18 class 14.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

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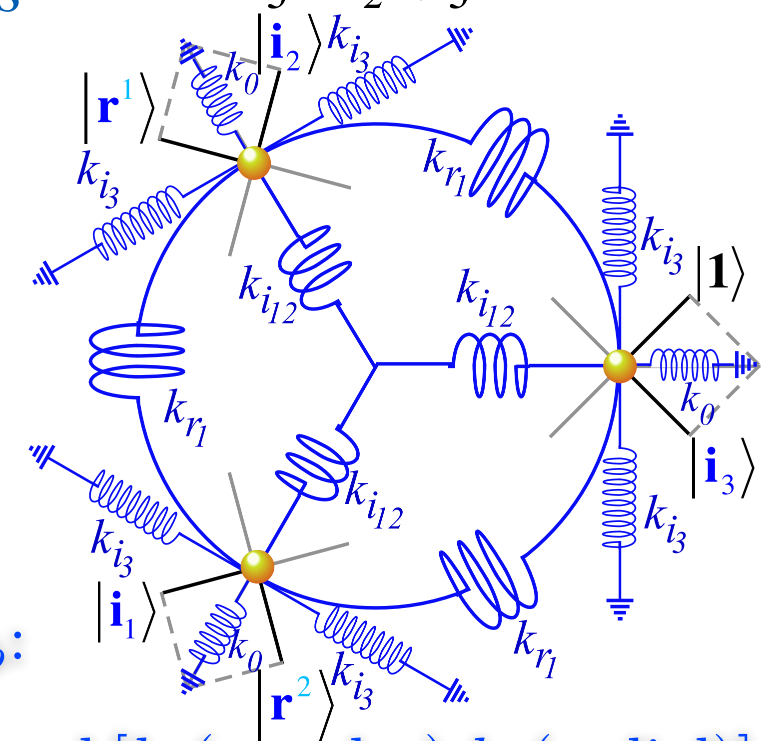
D_6 Band structure and related Global vs Local induced representations, *D_4 example*

U(12)-Supersymmetry

$D_3 \supset C_2(i_3)$ local-symmetry vibrational K-matrix eigensolutions



Generic **K**-*matrix (Top row)*

$$\langle \mathbf{1}|\mathbf{K}|\mathbf{g}_b\rangle = \begin{bmatrix} r_0 & r_1 & r_2 & i_1 & i_2 & i_3 \end{bmatrix}$$

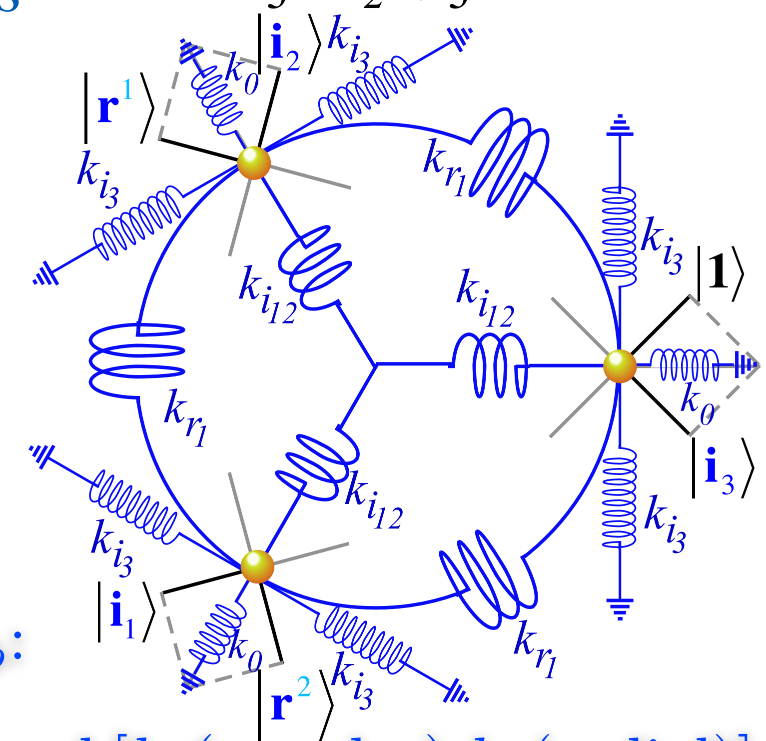
$D_3 \supset C_2(i_3)$ local-symmetry vibrational K-matrix

1^{st}-row parameters $g_b = \langle \mathbf{1}|\mathbf{K}|\mathbf{g}_b\rangle = K_{1b}$ of the force matrix K_{ab}:

$D_3 \supset C_2(i_3)$ model has internal [k_r(angular),k_i(radial)] and external [k_3(angular),k_0(radial)] constants between masses and lab frame.

$D_3 \supset C_2(i_3)$ local-symmetry vibrational K-matrix eigensolutions

Local D_3 $C_2 \supset (i_3)$ model



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$\lvert g_b\rangle$	$\lvert\mathbf{1}\rangle$	$\lvert\mathbf{r}^1\rangle$	$\lvert\mathbf{r}^2\rangle$	$\lvert\mathbf{i}_1\rangle$	$\lvert\mathbf{i}_2\rangle$	$\lvert\mathbf{i}_3\rangle$
$\langle \mathbf{1}\rvert\, \mathbf{K}\, \lvert g_b\rangle =$	$k_i/2$ $+k_r$ $+k_3$ $+k_0/2$	$k_i/2$ $-k_r/2$ $+0$ $+0$	$k_i/2$ $-k_r/2$ $+0$ $+0$	$k_i/2$ $+k_r/2$ $+0$ $+0$	$k_i/2$ $+k_r/2$ $+0$ $+0$	$k_i/2$ $-k_r$ $-k_3$ $+k_0/2$

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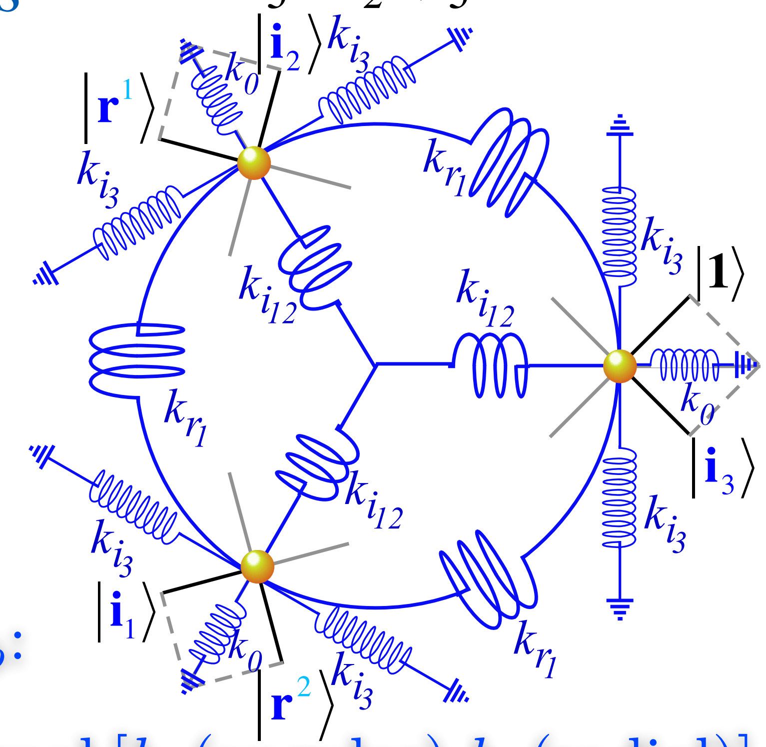
Local D_3 $C_2 \supset (i_3)$ model



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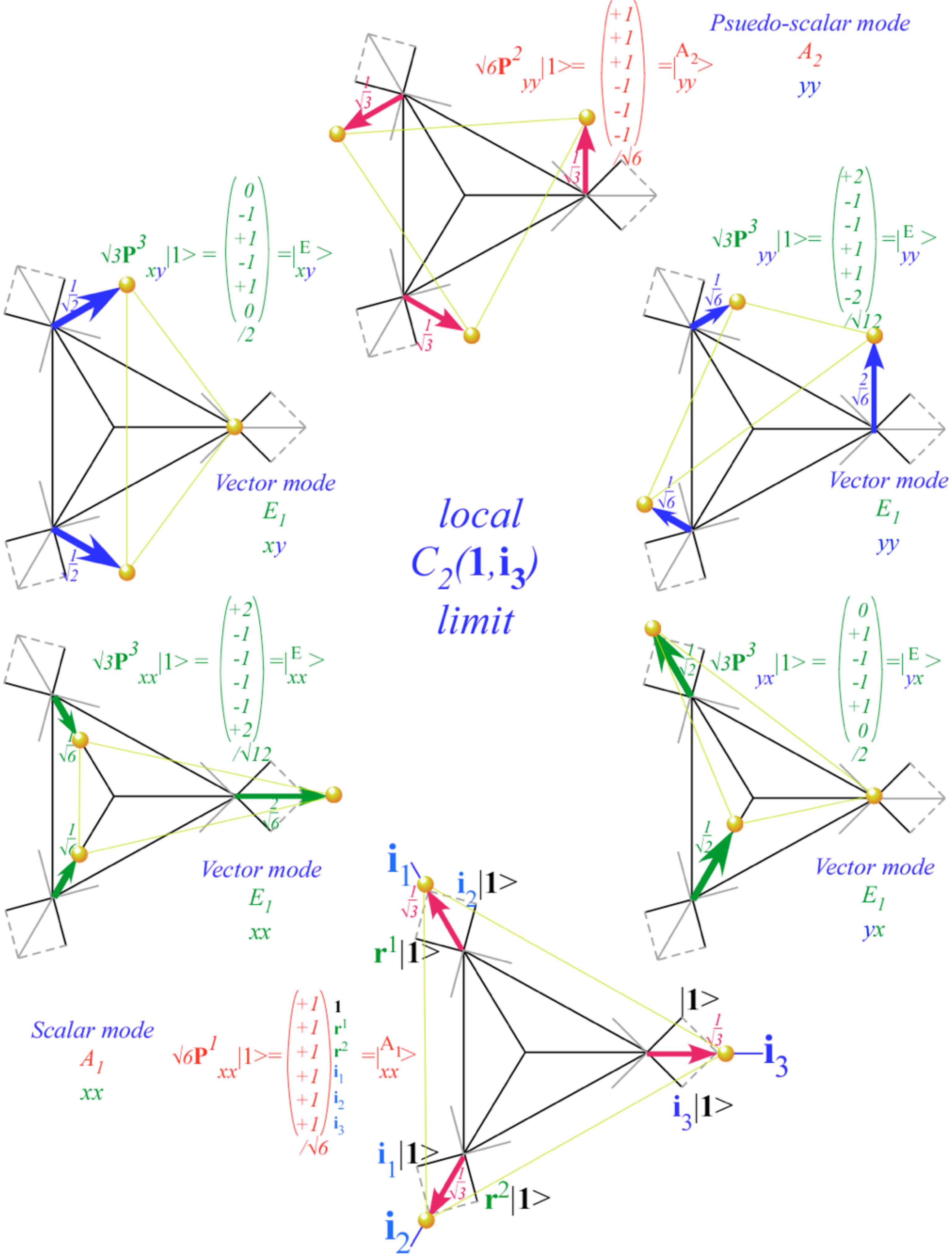
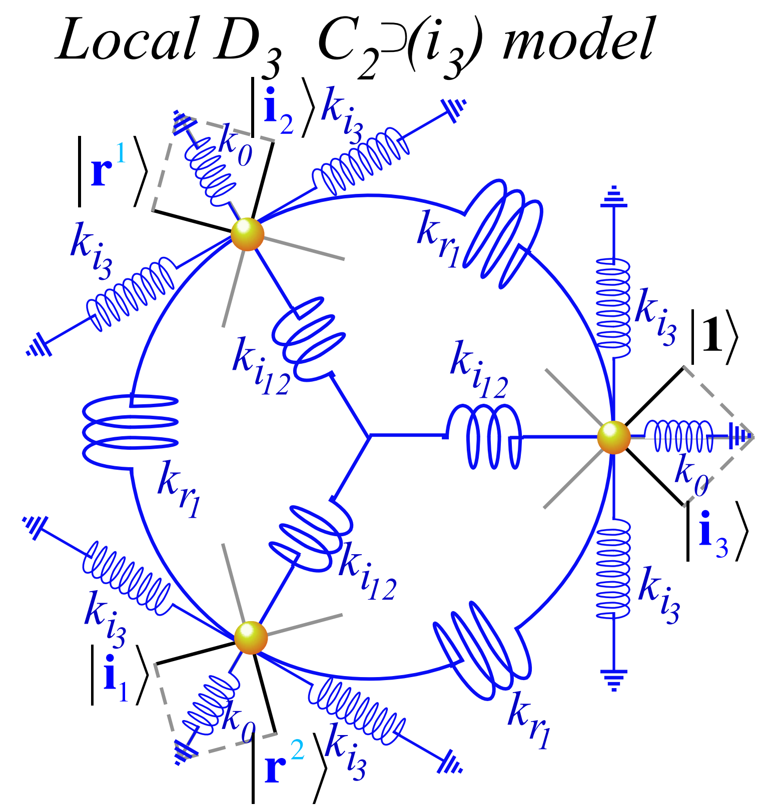
$D_3 \supset C_2(i_3)$ local-symmetry vibrational K-matrix eigenvalues $K_m/M = \omega_m^2$

$$K^{A_1}_{xx} = r_0 + r_1 + r_1^* + i_1 + i_2 + i_3 = k_0 + 3k_i$$

$$K^{A_2}_{yy} = r_0 + r_1 + r_1^* - i_1 - i_2 - i_3 = 3k_3$$

$$\begin{pmatrix} K^{E_1}_{xx} & K^{E_1}_{xy} \\ K^{E_1}_{yx} & K^{E_1}_{yy} \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 2r_0 - r_1 - r_1^* - i_1 - i_2 + 2i_3 & \sqrt{3}(-r_1 + r_1^* - i_1 + i_2) \\ \sqrt{3}(-r_1^* + r_1 - i_1 + i_2) & 2r_0 - r_1 - r_1^* + i_1 + i_2 - 2i_3 \end{pmatrix} = \begin{pmatrix} k_0 & 0 \\ 0 & k_3 + 2k_r \end{pmatrix}$$





Classical D_3 K-eigen-modes analogous to Quantum H-eigenwaves on following page

K-matrix symmetry analogous to quantum H-matrix

Global (LAB) symmetry

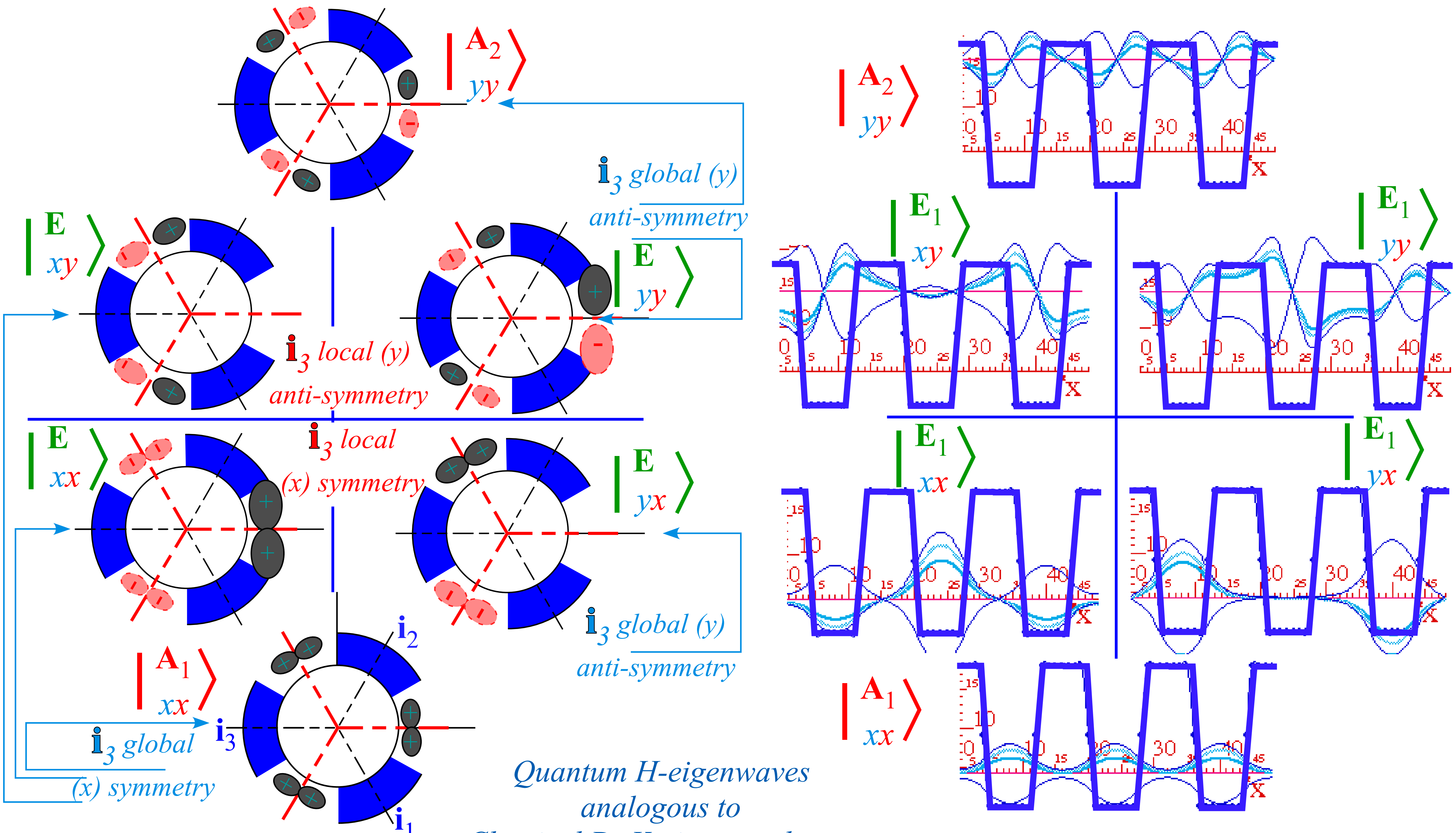
$$\mathbf{i}_3\left|{}^{(m)}_{eb}\right\rangle = \mathbf{i}_3\mathbf{P}^{(m)}_{eb}\left|1\right\rangle$$
$$= (-1)^e \left|{}^{(m)}\right\rangle$$

$D_3 > C_2\, \mathbf{i}_3$ *projector states*

$$\left|{}^{(m)}_{eb}\right\rangle = \mathbf{P}^{(m)}_{eb}\left|1\right\rangle$$

Local (BOD) symmetry

$$\bar{\mathbf{i}}_3\left|{}^{(m)}_{eb}\right\rangle = \bar{\mathbf{i}}_3\mathbf{P}^{(m)}_{eb}\left|1\right\rangle = \mathbf{P}^{(m)}_{eb}\bar{\mathbf{i}}_3\left|1\right\rangle$$
$$= \mathbf{P}^{(m)}_{eb}\mathbf{i}_3^{\dagger}\left|1\right\rangle = (-1)^b \left|{}^{(m)}\right\rangle$$



Quantum H-eigenwaves analogous to Classical D₃ K-eigen-modes on preceding page

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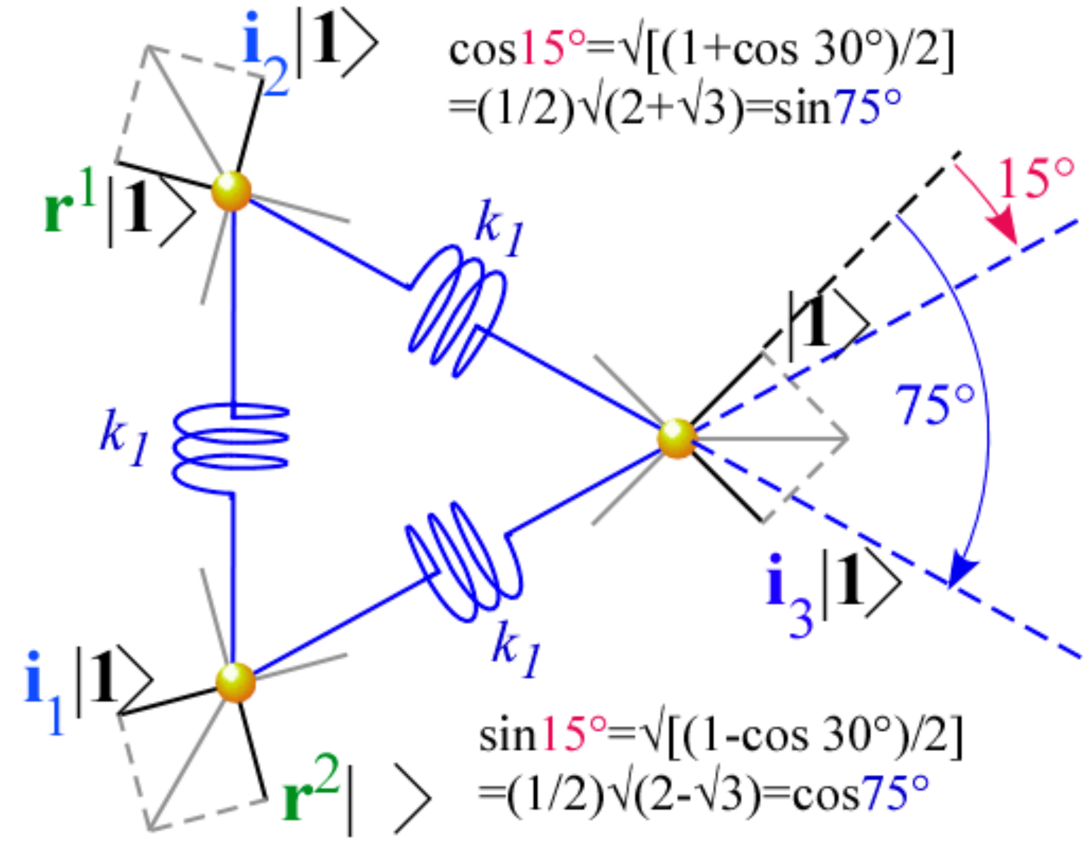

D_3-direct-connection vibrational K-matrix

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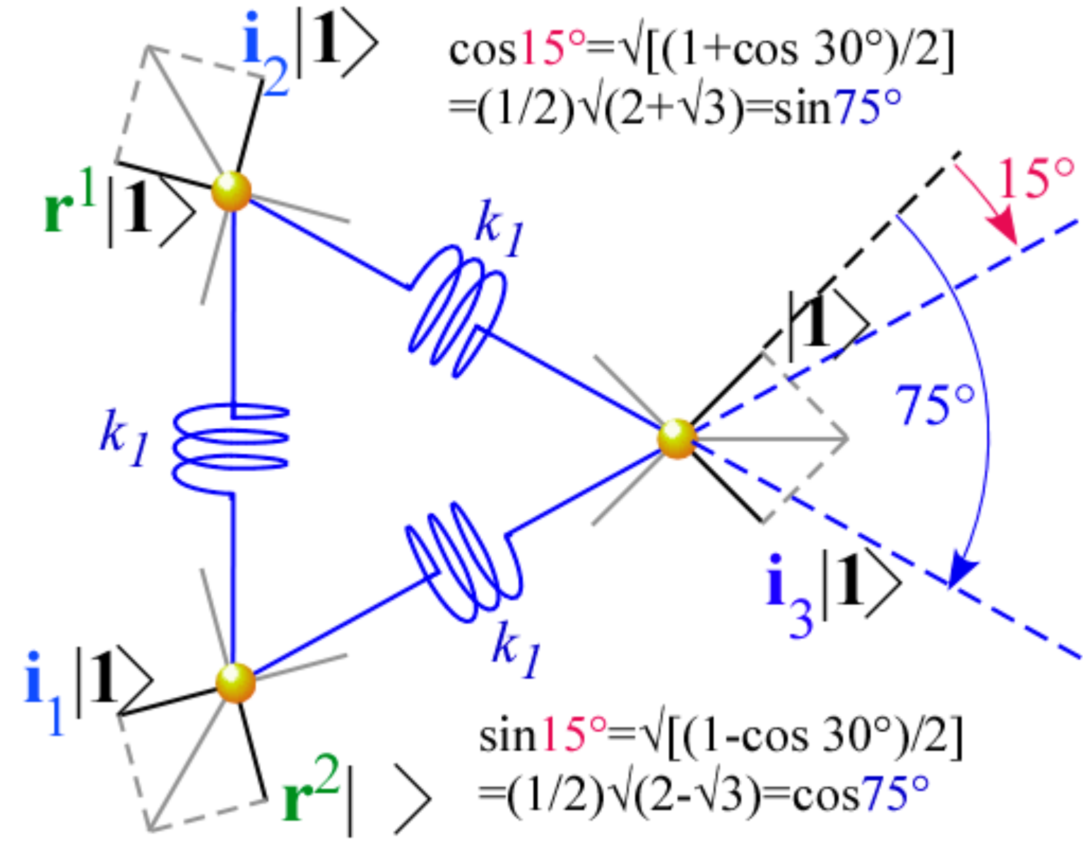
Generic **K**-matrix D_3 projections

$$K_{xx}^{A_1} = r_0 + r_1 + r_1^* + i_1 + i_2 + i_3$$

$$K_{yy}^{A_2} = r_0 + r_1 + r_1^* - i_1 - i_2 - i_3$$

$$\begin{pmatrix} K_{xx}^{E_1} & K_{xy}^{E_1} \\ K_{yx}^{E_1} & K_{yy}^{E_1} \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 2r_0 - r_1 - r_1^* - i_1 - i_2 + 2i_3 & \sqrt{3}(-r_1 + r_1^* - i_1 + i_2) \\ \sqrt{3}(-r_1^* + r_1 - i_1 + i_2) & 2r_0 - r_1 - r_1^* + i_1 + i_2 - 2i_3 \end{pmatrix}$$

D_3-direct-connection vibrational K-matrix



D_3-direct-connection K-matrix eigensolutions

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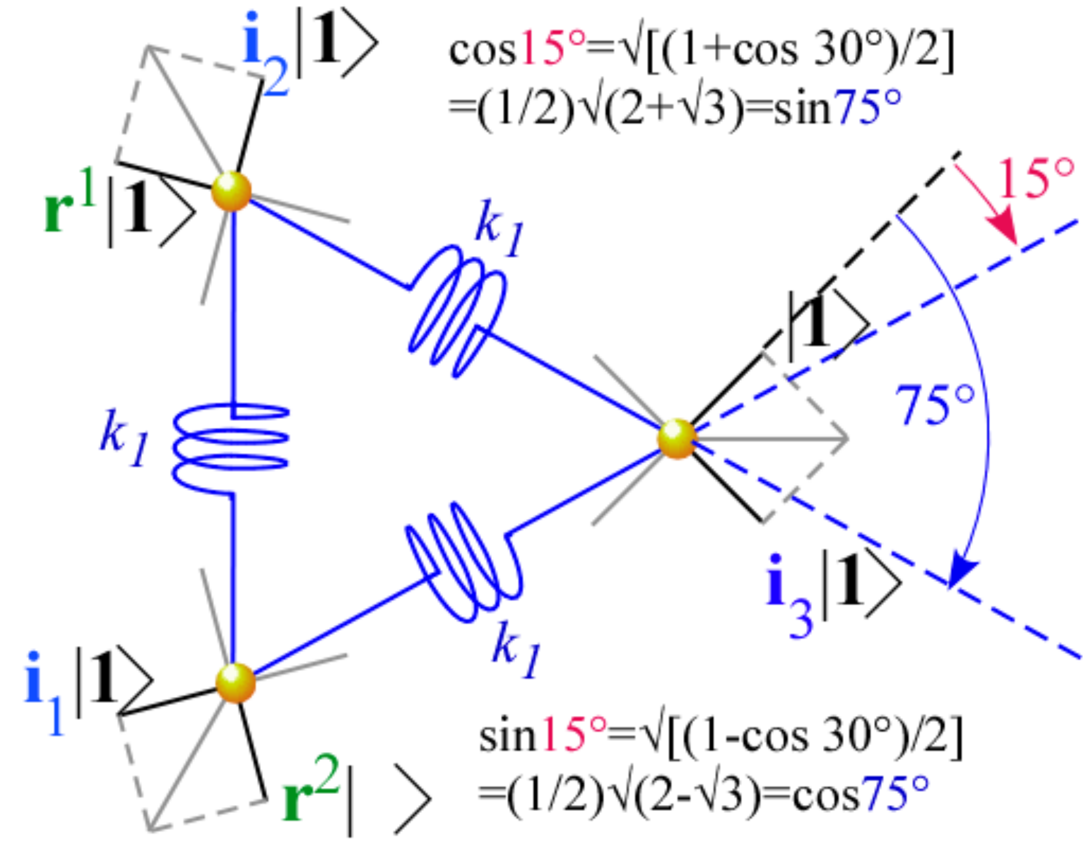


D_3-direct-connection vibrational K-matrix

$\lvert g_b\rangle$	$\lvert\mathbf{1}\rangle$	$\lvert\mathbf{r}^1\rangle$	$\lvert\mathbf{r}^2\rangle$	$\lvert\mathbf{i}_1\rangle$	$\lvert\mathbf{i}_2\rangle$	$\lvert\mathbf{i}_3\rangle$
$\langle\mathbf{1}\lvert\mathbf{K}\rvert g_b\rangle =$	$k_1(\cos^2 75° + \cos^2 15°) = k_1$	$k_1 \cos 75° \cdot \cos 15° = \frac{k_1}{4}$	$k_1 \cos 15° \cdot \cos 75° = \frac{k_1}{4}$	$k_1 \cos 15° \cdot \cos 15° = \frac{k_1(2-\sqrt{3})}{4}$	$k_1 \cos 75° \cdot \cos 75° = \frac{k_1(2+\sqrt{3})}{4}$	$k_1(\cos^2 75° - \cos^2 15°) = \frac{k_1}{2}$

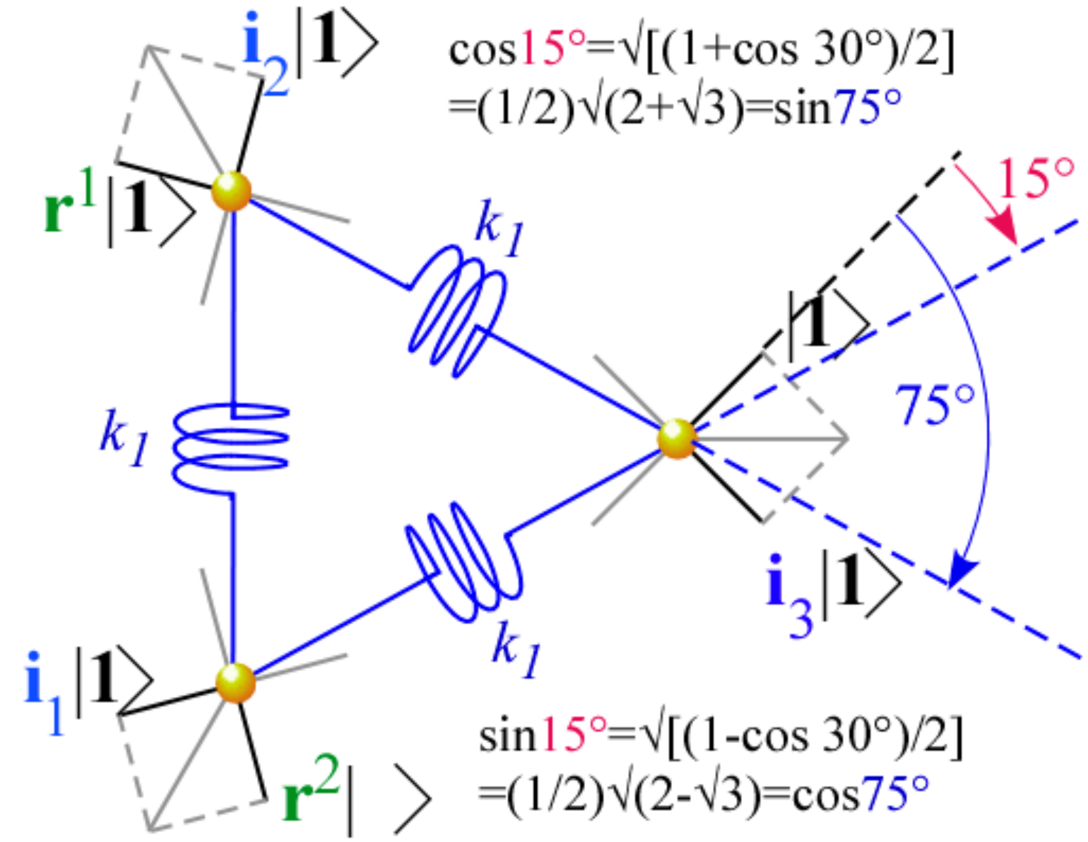
D_3-direct-connection K-matrix eigensolutions

Generic **K**-matrix (Top row)

$$\langle \mathbf{1}|\mathbf{K}|\mathbf{g}_b\rangle = \begin{bmatrix} r_0 & r_1 & r_2 & i_1 & i_2 & i_3 \end{bmatrix}$$

Generic **K**-matrix D_3 projections

$$K^{A_1}_{xx} = r_0+r_1+r_1^*+i_1+i_2+i_3$$
$$K^{A_2}_{yy} = r_0+r_1+r_1^*-i_1-i_2-i_3$$
$$\begin{pmatrix} K^{E_1}_{xx} & K^{E_1}_{xy} \\ K^{E_1}_{yx} & K^{E_1}_{yy} \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 2r_0-r_1-r_1^*-i_1-i_2+2i_3 & \sqrt{3}(-r_1+r_1^*-i_1+i_2) \\ \sqrt{3}(-r_1^*+r_1-i_1+i_2) & 2r_0-r_1-r_1^*+i_1+i_2-2i_3 \end{pmatrix}$$



D_3-direct-connection vibrational K-matrix

$\|g_b\rangle$	$\|\mathbf{1}\rangle$	$\|\mathbf{r}^1\rangle$	$\|\mathbf{r}^2\rangle$	$\|\mathbf{i}_1\rangle$	$\|\mathbf{i}_2\rangle$	$\|\mathbf{i}_3\rangle$
$\langle\mathbf{1}\|\mathbf{K}\|g_b\rangle =$	$k_1(\cos^2 75° + \cos^2 15°) = k_1$	$k_1 \cos 75° \cdot \cos 15° = \frac{k_1}{4}$	$k_1 \cos 15° \cdot \cos 75° = \frac{k_1}{4}$	$k_1 \cos 15° \cdot \cos 15° = \frac{k_1(2-\sqrt{3})}{4}$	$k_1 \cos 75° \cdot \cos 75° = \frac{k_1(2+\sqrt{3})}{4}$	$k_1(\cos^2 75° - \cos^2 15°) = \frac{k_1}{2}$

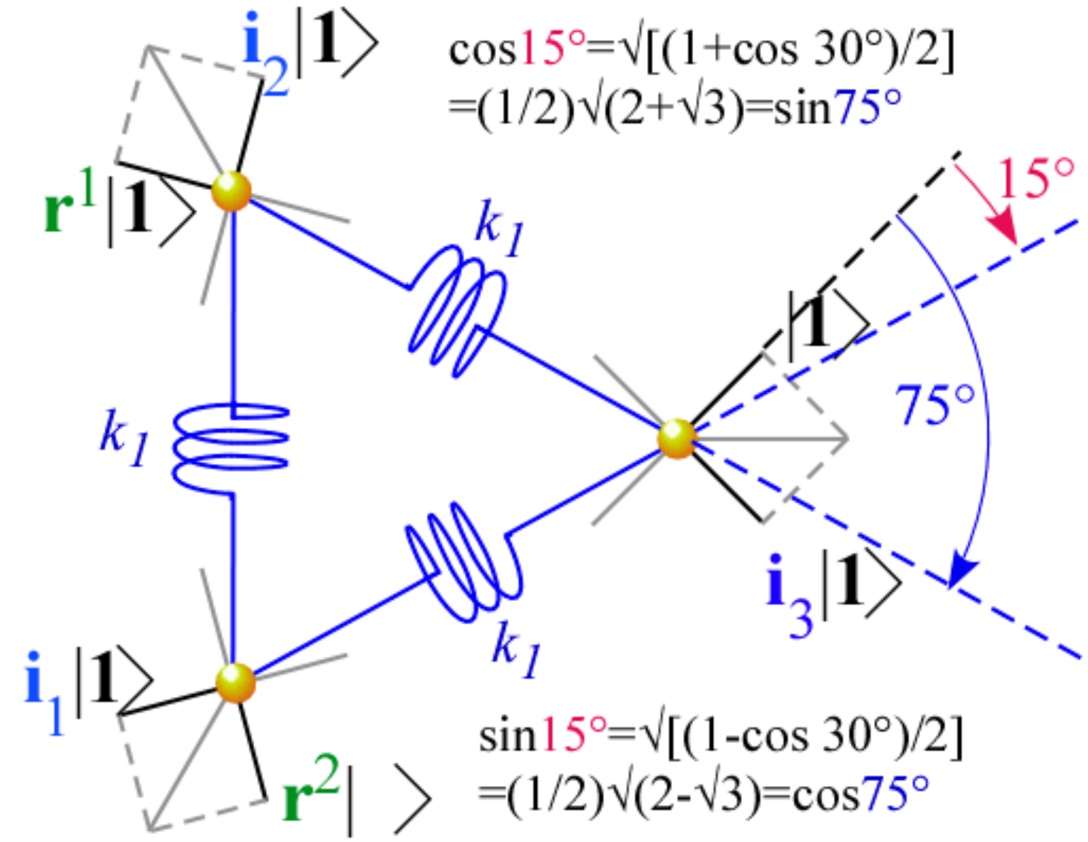
$$K^{A_1}_{xx} = r_0+r_1+r_1^*+i_1+i_2+i_3$$
$$K^{A_2}_{yy} = r_0+r_1+r_1^*-i_1-i_2-i_3$$
$$\begin{pmatrix} K^{E_1}_{xx} & K^{E_1}_{xy} \\ K^{E_1}_{yx} & K^{E_1}_{yy} \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 2r_0-r_1-r_1^*-i_1-i_2+2i_3 & \sqrt{3}(-r_1+r_1^*-i_1+i_2) \\ \sqrt{3}(-r_1^*+r_1-i_1+i_2) & 2r_0-r_1-r_1^*+i_1+i_2-2i_3 \end{pmatrix}$$

$$= k_1+\frac{k_1}{4}+\frac{k_1}{4}+\frac{k_1}{2}+\frac{k_1}{2}+\frac{k_1}{2} = \frac{3k_1}{2}+\frac{3k_1}{2} = 3k_1$$
$$= k_1+\frac{k_1}{4}+\frac{k_1}{4}-\frac{k_1}{2}-\frac{k_1}{2}-\frac{k_1}{2} = \frac{3k_1}{2}-\frac{3k_1}{2} = 0$$

D_3-direct-connection K-matrix eigensolutions

Generic **K**-matrix (Top row)

$$\langle \mathbf{1}|\mathbf{K}|\mathbf{g}_b\rangle = \begin{bmatrix} r_0 & r_1 & r_2 & i_1 & i_2 & i_3 \end{bmatrix}$$



Generic **K**-matrix D_3 projections

$$K^{A_1}_{xx} = r_0 + r_1 + r_1^* + i_1 + i_2 + i_3$$
$$K^{A_2}_{yy} = r_0 + r_1 + r_1^* - i_1 - i_2 - i_3$$
$$\begin{pmatrix} K^{E_1}_{xx} & K^{E_1}_{xy} \\ K^{E_1}_{yx} & K^{E_1}_{yy} \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 2r_0 - r_1 - r_1^* - i_1 - i_2 + 2i_3 & \sqrt{3}(-r_1 + r_1^* - i_1 + i_2) \\ \sqrt{3}(-r_1^* + r_1 - i_1 + i_2) & 2r_0 - r_1 - r_1^* + i_1 + i_2 - 2i_3 \end{pmatrix}$$

D_3-direct-connection vibrational K-matrix

$\lvert g_b\rangle$	$\lvert\mathbf{1}\rangle$	$\lvert\mathbf{r}^1\rangle$	$\lvert\mathbf{r}^2\rangle$	$\lvert\mathbf{i}_1\rangle$	$\lvert\mathbf{i}_2\rangle$	$\lvert\mathbf{i}_3\rangle$
$\langle\mathbf{1}\rvert\,\mathbf{K}\,\lvert g_b\rangle =$	$k_1(\cos^2 75^\circ + \cos^2 15^\circ) = k_1$	$k_1 \cos 75^\circ \cdot \cos 15^\circ = \frac{k_1}{4}$	$k_1 \cos 15^\circ \cdot \cos 75^\circ = \frac{k_1}{4}$	$k_1 \cos 15^\circ \cdot \cos 15^\circ = \frac{k_1(2-\sqrt{3})}{4}$	$k_1 \cos 75^\circ \cdot \cos 75^\circ = \frac{k_1(2+\sqrt{3})}{4}$	$k_1(\cos^2 75^\circ - \cos^2 15^\circ) = \frac{k_1}{2}$

$$K^{A_1}_{xx} = r_0 + r_1 + r_1^* + i_1 + i_2 + i_3 = k_1 + \frac{k_1}{4} + \frac{k_1}{4} + \frac{k_1}{2} + \frac{k_1}{2} + \frac{k_1}{2} = \frac{3k_1}{2} + \frac{3k_1}{2} = 3k_1$$
$$K^{A_2}_{yy} = r_0 + r_1 + r_1^* - i_1 - i_2 - i_3 = k_1 + \frac{k_1}{4} + \frac{k_1}{4} - \frac{k_1}{2} - \frac{k_1}{2} - \frac{k_1}{2} = \frac{3k_1}{2} - \frac{3k_1}{2} = 0$$
$$\begin{pmatrix} K^{E_1}_{xx} & K^{E_1}_{xy} \\ K^{E_1}_{yx} & K^{E_1}_{yy} \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 2r_0 - r_1 - r_1^* - i_1 - i_2 + 2i_3 & \sqrt{3}(-r_1 + r_1^* - i_1 + i_2) \\ \sqrt{3}(-r_1^* + r_1 - i_1 + i_2) & 2r_0 - r_1 - r_1^* + i_1 + i_2 - 2i_3 \end{pmatrix}$$

$$\begin{pmatrix} \frac{1}{2}\left(2k_1 - \frac{k_1}{4} - \frac{k_1}{4} - \frac{k_1}{2} - \frac{k_1}{2} + 2\frac{k_1}{2}\right) = \frac{1}{2}\left(2k_1 - \frac{k_1}{2} - k_1 + k_1\right) = \frac{3k_1}{4} & \text{(symmetric)} \\ \frac{\sqrt{3}}{2}\left(-\frac{k_1}{4} + \frac{k_1}{4} + \frac{k_1\sqrt{3}}{4} + \frac{k_1\sqrt{3}}{4}\right) = \frac{k_1 3}{4} & \frac{1}{2}\left(2k_1 - \frac{k_1}{4} - \frac{k_1}{4} + \frac{k_1}{2} + \frac{k_1}{2} - 2\frac{k_1}{2}\right) = \frac{3k_1}{4} \end{pmatrix}$$

D_3-direct-connection K-matrix eigensolutions

Generic **K**-matrix (Top row)

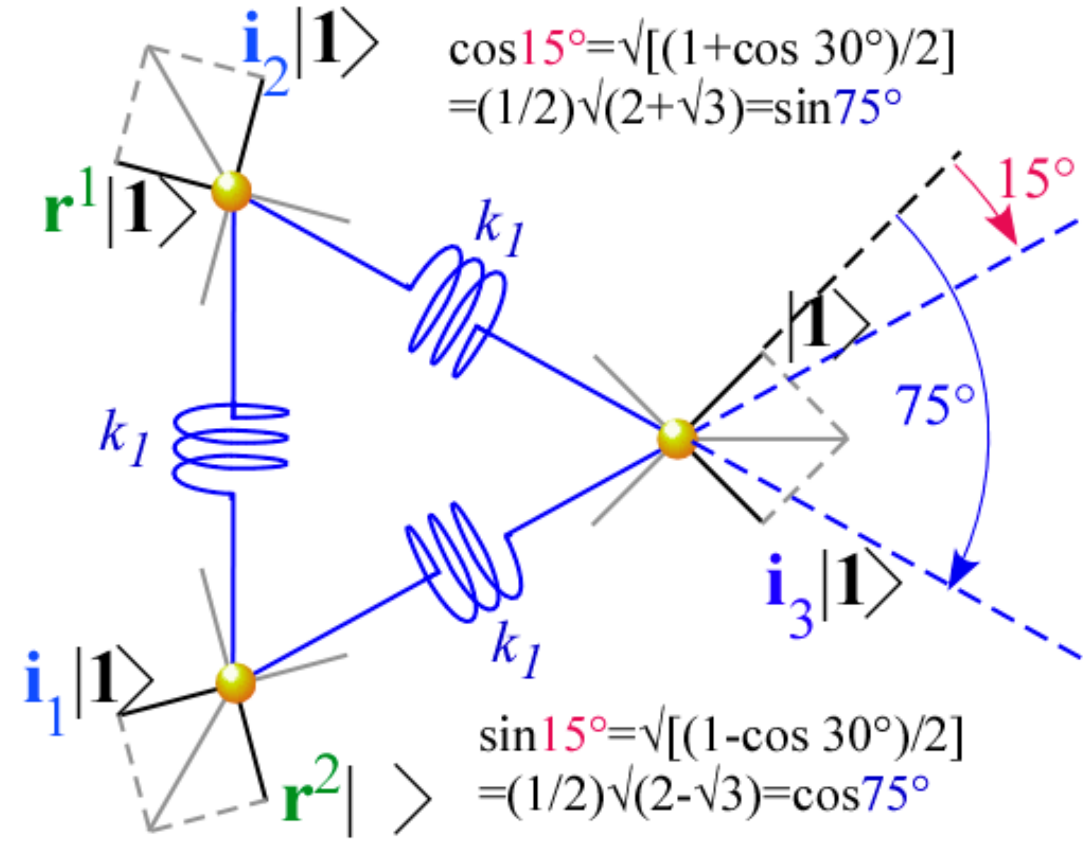
$$\langle \mathbf{1} | \mathbf{K} | \mathbf{g}_b \rangle = \begin{bmatrix} r_0 & r_1 & r_2 & i_1 & i_2 & i_3 \end{bmatrix}$$

Generic **K**-matrix D_3 projections

$$K_{xx}^{A_1} = r_0 + r_1 + r_1^* + i_1 + i_2 + i_3$$

$$K_{yy}^{A_2} = r_0 + r_1 + r_1^* - i_1 - i_2 - i_3$$

$$\begin{pmatrix} K_{xx}^{E_1} & K_{xy}^{E_1} \\ K_{yx}^{E_1} & K_{yy}^{E_1} \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 2r_0 - r_1 - r_1^* - i_1 - i_2 + 2i_3 & \sqrt{3}(-r_1 + r_1^* - i_1 + i_2) \\ \sqrt{3}(-r_1^* + r_1 - i_1 + i_2) & 2r_0 - r_1 - r_1^* + i_1 + i_2 - 2i_3 \end{pmatrix}$$



D_3-direct-connection vibrational K-matrix

$\vert g_b\rangle$	$\vert\mathbf{1}\rangle$	$\vert\mathbf{r}^1\rangle$	$\vert\mathbf{r}^2\rangle$	$\vert\mathbf{i}_1\rangle$	$\vert\mathbf{i}_2\rangle$	$\vert\mathbf{i}_3\rangle$
$\langle \mathbf{1} \vert \mathbf{K} \vert g_b \rangle =$	$k_1(\cos^2 75° + \cos^2 15°) = k_1$	$k_1 \cos 75° \cdot \cos 15° = \frac{k_1}{4}$	$k_1 \cos 15° \cdot \cos 75° = \frac{k_1}{4}$	$k_1 \cos 15° \cdot \cos 15° = \frac{k_1(2-\sqrt{3})}{4}$	$k_1 \cos 75° \cdot \cos 75° = \frac{k_1(2+\sqrt{3})}{4}$	$k_1(\cos^2 75° - \cos^2 15°) = \frac{k_1}{2}$

D_3-direct-connection vibrational K-matrix eigenvalues $K_m/M=\omega_m^2$

$$K_{xx}^{A_1} = 3k_1$$

$$K_{yy}^{A_2} = 0$$

$$\begin{pmatrix} K_{xx}^{E_1} & K_{xy}^{E_1} \\ K_{yx}^{E_1} & K_{yy}^{E_1} \end{pmatrix} = \begin{pmatrix} \frac{3k_1}{4} & \frac{3k_1}{4} \\ \frac{3k_1}{4} & \frac{3k_1}{4} \end{pmatrix}$$

D_3-direct-connection K-matrix eigensolutions

Generic K-matrix (Top row)

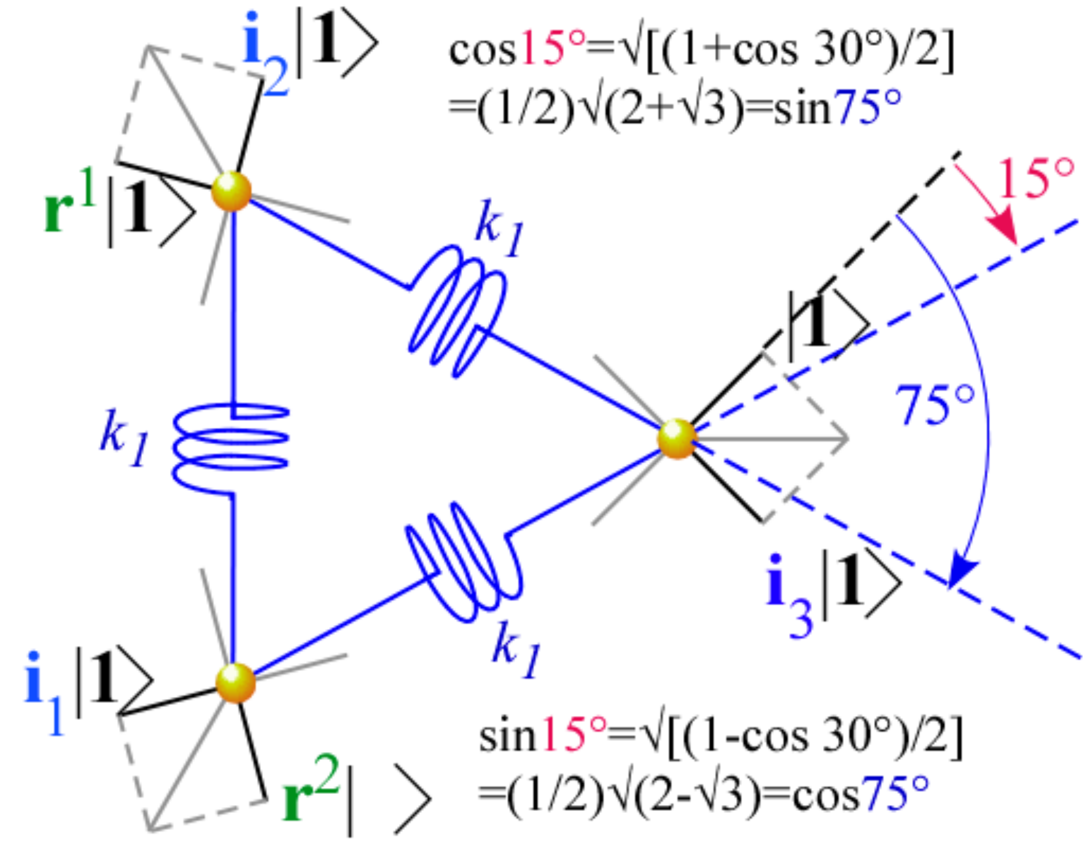
$$\langle \mathbf{1}|\mathbf{K}|\mathbf{g}_b\rangle = \begin{bmatrix} r_0 & r_1 & r_2 & i_1 & i_2 & i_3 \end{bmatrix}$$

Generic K-matrix D_3 projections

$$K^{A_1}_{xx} = r_0 + r_1 + r_1^* + i_1 + i_2 + i_3$$

$$K^{A_2}_{yy} = r_0 + r_1 + r_1^* - i_1 - i_2 - i_3$$

$$\begin{pmatrix} K^{E_1}_{xx} & K^{E_1}_{xy} \\ K^{E_1}_{yx} & K^{E_1}_{yy} \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 2r_0 - r_1 - r_1^* - i_1 - i_2 + 2i_3 & \sqrt{3}(-r_1 + r_1^* - i_1 + i_2) \\ \sqrt{3}(-r_1^* + r_1 - i_1 + i_2) & 2r_0 - r_1 - r_1^* + i_1 + i_2 - 2i_3 \end{pmatrix}$$



D_3-direct-connection vibrational K-matrix

$\lvert g_b\rangle$	$\lvert\mathbf{1}\rangle$	$\lvert\mathbf{r}^1\rangle$	$\lvert\mathbf{r}^2\rangle$	$\lvert\mathbf{i}_1\rangle$	$\lvert\mathbf{i}_2\rangle$	$\lvert\mathbf{i}_3\rangle$
$\langle\mathbf{1}\rvert\,\mathbf{K}\,\lvert g_b\rangle =$	$k_1(\cos^2 75^\circ + \cos^2 15^\circ) = k_1$	$k_1 \cos 75^\circ \cdot \cos 15^\circ = \frac{k_1}{4}$	$k_1 \cos 15^\circ \cdot \cos 75^\circ = \frac{k_1}{4}$	$k_1 \cos 15^\circ \cdot \cos 15^\circ = \frac{k_1(2-\sqrt{3})}{4}$	$k_1 \cos 75^\circ \cdot \cos 75^\circ = \frac{k_1(2+\sqrt{3})}{4}$	$k_1(\cos^2 75^\circ - \cos^2 15^\circ) = \frac{k_1}{2}$

D_3-direct-connection vibrational K-matrix eigenvalues $K_m/M=\omega_m^2$

$$K^{A_1}_{xx} = 3k_1$$

$$K^{A_2}_{yy} = 0$$

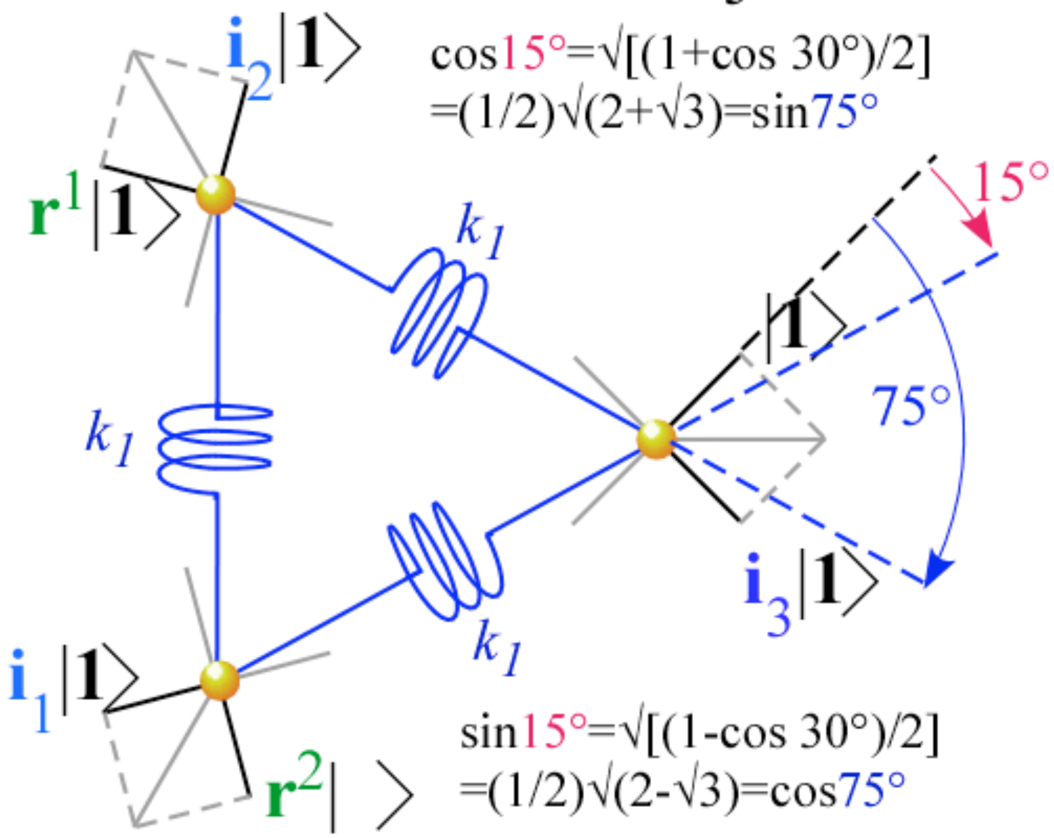
$$\begin{pmatrix} K^{E_1}_{xx} & K^{E_1}_{xy} \\ K^{E_1}_{yx} & K^{E_1}_{yy} \end{pmatrix} = \begin{pmatrix} \frac{3k_1}{4} & \frac{3k_1}{4} \\ \frac{3k_1}{4} & \frac{3k_1}{4} \end{pmatrix}$$

E_1 Eigenvectors in terms of $D_3 \supset C_2(i_3)$ E_1-vectors

$$\mathbf{K}\left|\begin{matrix} E_1 \\ g(+) \end{matrix}\right\rangle = \mathbf{K}\left(\left|\begin{matrix} E_1 \\ gx \end{matrix}\right\rangle + \left|\begin{matrix} E_1 \\ gy \end{matrix}\right\rangle\right)\frac{1}{\sqrt{2}} = \frac{3k_1}{2}\left|\begin{matrix} E_1 \\ g(+) \end{matrix}\right\rangle,$$

$$\mathbf{K}\left|\begin{matrix} E_1 \\ g(-) \end{matrix}\right\rangle = \mathbf{K}\left(\left|\begin{matrix} E_1 \\ gx \end{matrix}\right\rangle - \left|\begin{matrix} E_1 \\ gy \end{matrix}\right\rangle\right)\frac{1}{\sqrt{2}} = 0\left|\begin{matrix} E_1 \\ g(-) \end{matrix}\right\rangle, \quad g = (x \text{ or } y).$$

Mixed local symmetry D_3 model



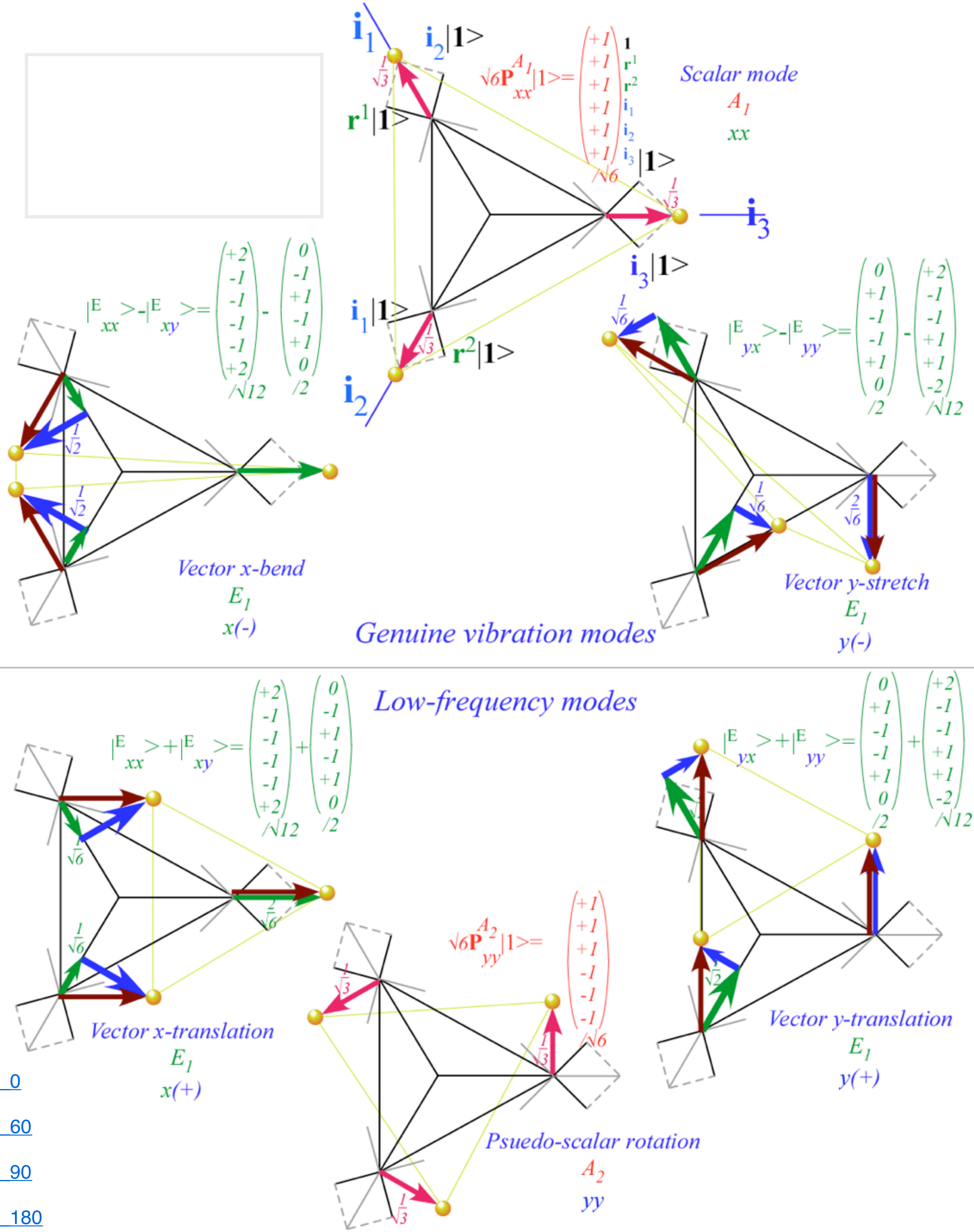
$\cos 15° = \sqrt{[(1+\cos 30°)/2]}$
$= (1/2)\sqrt{(2+\sqrt{3})} = \sin 75°$

$\sin 15° = \sqrt{[(1-\cos 30°)/2]}$
$= (1/2)\sqrt{(2-\sqrt{3})} = \cos 75°$

$$K^{A_1}_{xx} = 3k_1$$

$$K^{A_2}_{yy} = 0$$

$$\begin{pmatrix} K^{E_1}_{xx} & K^{E_1}_{xy} \\ K^{E_1}_{yx} & K^{E_1}_{yy} \end{pmatrix} = \begin{pmatrix} \frac{3k_1}{4} & \frac{3k_1}{4} \\ \frac{3k_1}{4} & \frac{3k_1}{4} \end{pmatrix}$$



https://modphys.hosted.uark.edu/markup/MolVibesWeb.html?scenario=C3vN3

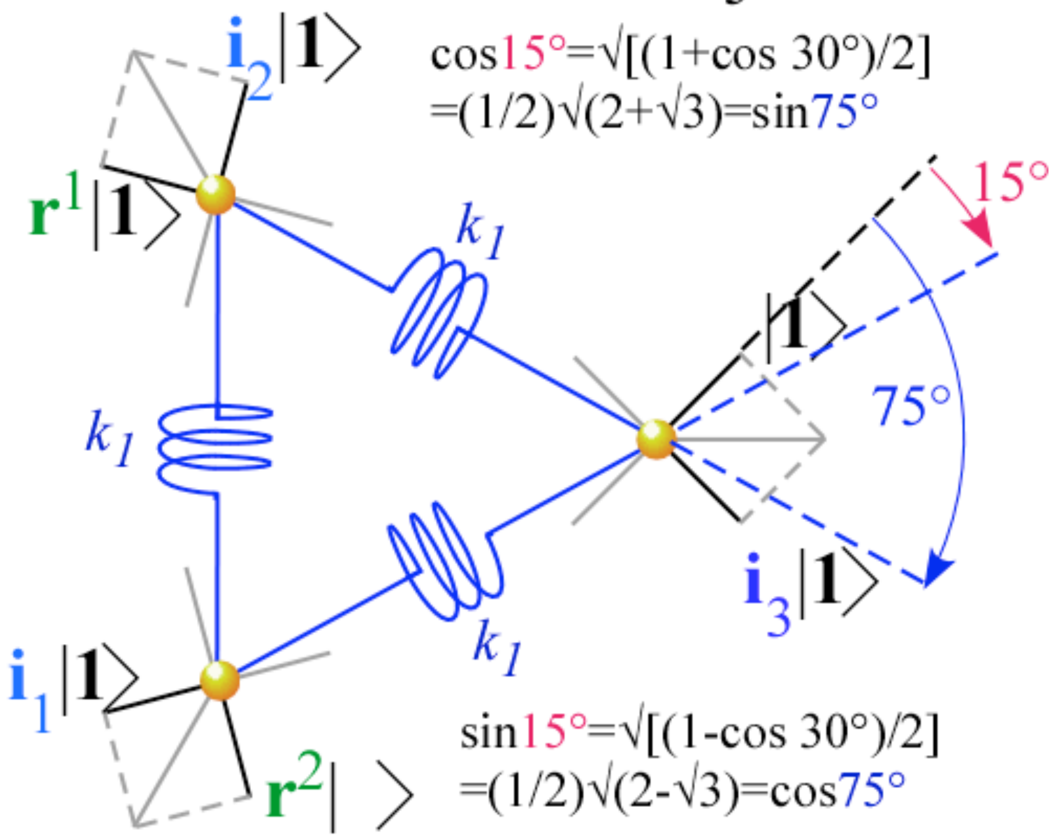
https://modphys.hosted.uark.edu/markup/MolVibesWeb.html?scenario=C3vN3_0

https://modphys.hosted.uark.edu/markup/MolVibesWeb.html?scenario=C3vN3_60

https://modphys.hosted.uark.edu/markup/MolVibesWeb.html?scenario=C3vN3_90

https://modphys.hosted.uark.edu/markup/MolVibesWeb.html?scenario=C3vN3_180

Mixed local symmetry D_3 model



$\cos 15° = \sqrt{[(1+\cos 30°)/2]}$
$= (1/2)\sqrt{(2+\sqrt{3})} = \sin 75°$

$\sin 15° = \sqrt{[(1-\cos 30°)/2]}$
$= (1/2)\sqrt{(2-\sqrt{3})} = \cos 75°$

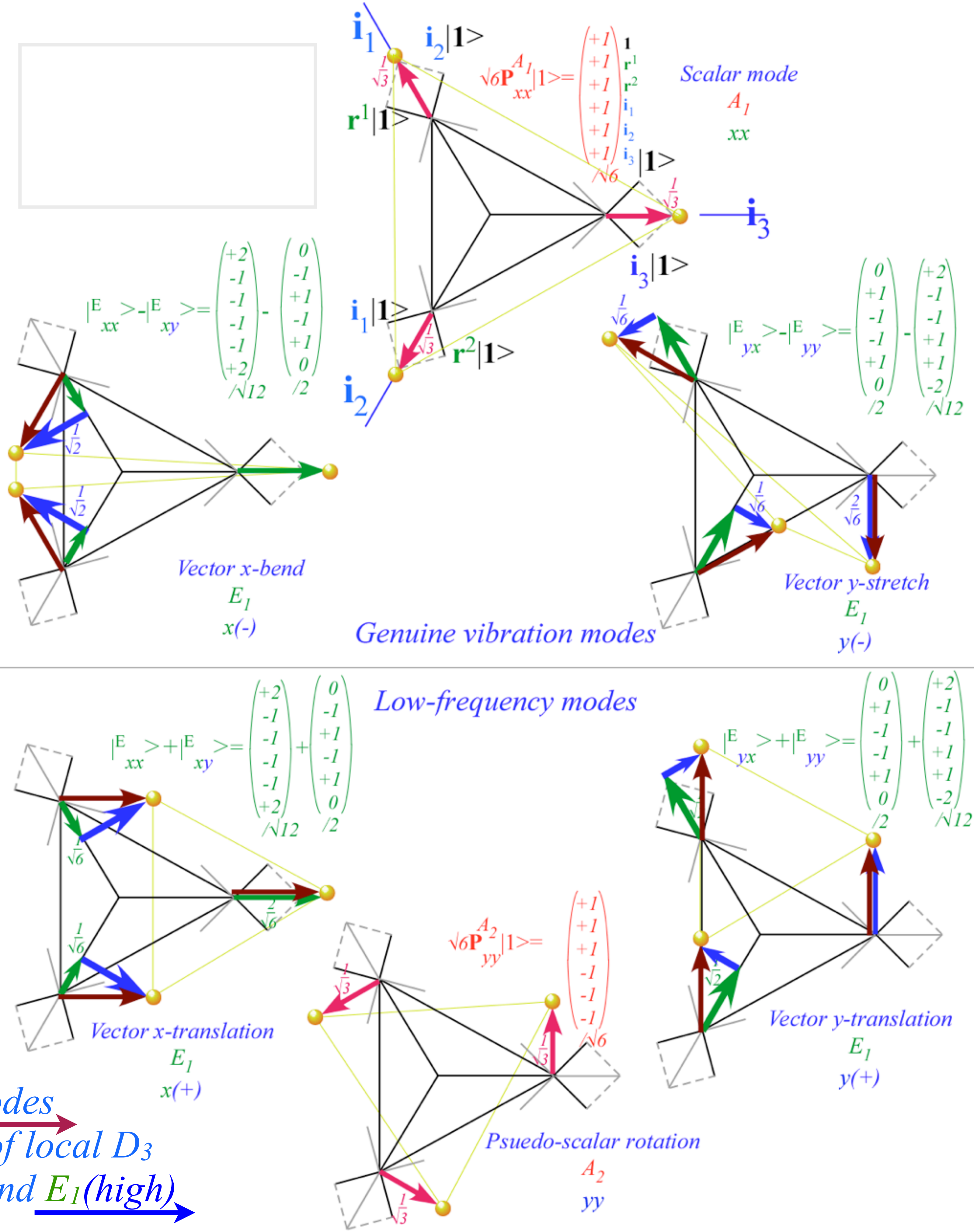
$$K^{A_1}_{xx} = 3k_1$$

$$K^{A_2}_{yy} = 0$$

$$\begin{pmatrix} K^{E_1}_{xx} & K^{E_1}_{xy} \\ K^{E_1}_{yx} & K^{E_1}_{yy} \end{pmatrix} = \begin{pmatrix} \frac{3k_1}{4} & \frac{3k_1}{4} \\ \frac{3k_1}{4} & \frac{3k_1}{4} \end{pmatrix}$$

E_1 Eigenvalues: $\frac{3k_1}{2}$ $\quad 0$

E_1 Eigenvectors: $\begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}$ $\begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{-1}{\sqrt{2}} \end{pmatrix}$



Mixed modes in terms of local D_3
E_1(low) and E_1(high)

AMOP reference links on page 2

2.26.18 class 14.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

Discrete symmetry subgroups of O(3) using Mock-Mach principle: $D_3 \sim C_{3v}$ LAB vs BOD
Vibrational eigensolutions, $D_6 \sim C_{6v}$ bands, subgroup correlation, and Frobenius reciprocity

Review: *H-matrix Global vs Local symmetry*

Molecular vibration K-matrix symmetry analogous to quantum H-matrix

Molecular K-matrix construction

$D_3 \supset C_2(i_3)$ local-symmetry K-matrix eigensolutions

D_3-direct-connection K-matrix eigenstates mix local symmetry

➡ *$D_3 \supset C_3(\mathbf{r}^{\pm 1})$ moving-wave local symmetry K-matrix "Coriolis" eigensolutions*

Applied symmetry reduction and splitting

Subduced irep $D^\alpha(D^3) \downarrow C_2 = d^{0_2} \oplus d^{1_2} \oplus$.. correlation

Subduced irep $D^\alpha(D^3) \downarrow C_3 = d^{0_3} \oplus d^{1_3} \oplus$.. correlation

Spontaneous symmetry breaking and clustering: Frobenius Reciprocity and band structure

Induced rep $d^a(C_2) \uparrow D^3 = D^\alpha \oplus D^\beta \oplus$.. correlation

Induced rep $d^a(C_3) \uparrow D^3 = D^\alpha \oplus D^\beta \oplus$.. correlation

D_6 symmetry and Hexagonal Bands

Cross product of the C_2 and D_3 characters gives all $D_6 = D_3 \times C_2$ characters and ireps

D_6 Band structure and related Global vs Local induced representations, *D_4 example*

U(12)-Supersymmetry

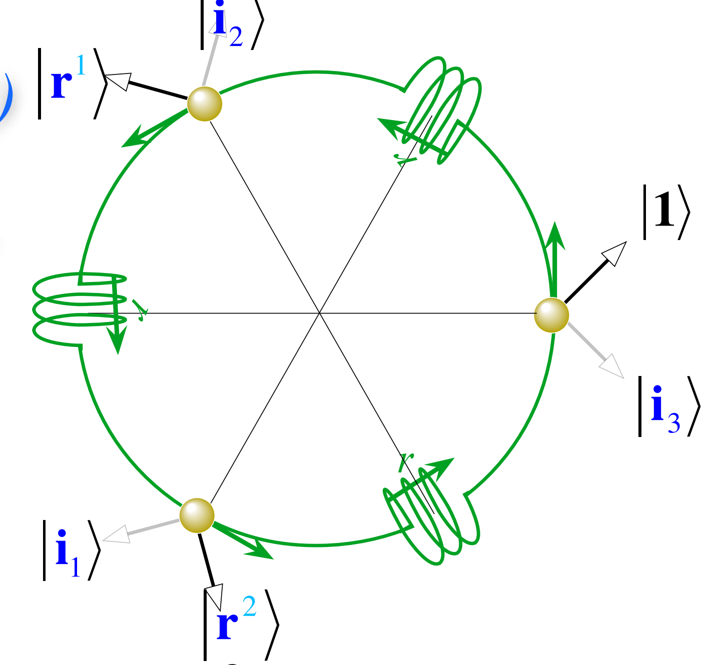
$D_3\supset C_3(\mathbf{r}^{\pm 1})$ local symmetry K-matrix eigensolutions

Generic **K**-matrix (Top row)

$$\langle\mathbf{1}|\mathbf{K}|\mathbf{g}_b\rangle = \begin{bmatrix} r_0 & r_1 & r_2 & i_1 & i_2 & i_3 \end{bmatrix}$$

$$\langle\mathbf{1}|\mathbf{K}_{C_3}|\mathbf{g}_b\rangle = \begin{bmatrix} r_0 & ir & -ir & 0 & 0 & 0 \end{bmatrix}$$

$D_3\supset C_3(\mathbf{r}^{\pm 1})$ local symmetry model



$D_3\supset C_3(\mathbf{r}^{\pm 1})$ local symmetry vibrational K-matrix

Set: $r_1 = r = -r_2^*$, and: $i_1 = i_2 = i_3 = 0$

$$K_{xx}^{A_1} = r_0 + r_1 + r_1^* + i_1 + i_2 + i_3 = r_0$$

$$K_{yy}^{A_2} = r_0 + r_1 + r_1^* - i_1 - i_2 - i_3 = r_0$$

$$\begin{pmatrix} K_{xx}^{E_1} & K_{xy}^{E_1} \\ K_{yx}^{E_1} & K_{yy}^{E_1} \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 2r_0 - r_1 - r_1^* - i_1 - i_2 + 2i_3 & \sqrt{3}(-r_1 + r_1^* - i_1 + i_2) \\ \sqrt{3}(-r_1^* + r_1 - i_1 + i_2) & 2r_0 - r_1 - r_1^* + i_1 + i_2 - 2i_3 \end{pmatrix}_{\substack{r_1=r=-r_2^* \\ i_1=i_2=i_3=0}} = \begin{pmatrix} r_0 & -ir\frac{\sqrt{3}}{2} \\ +ir\frac{\sqrt{3}}{2} & r_0 \end{pmatrix}$$

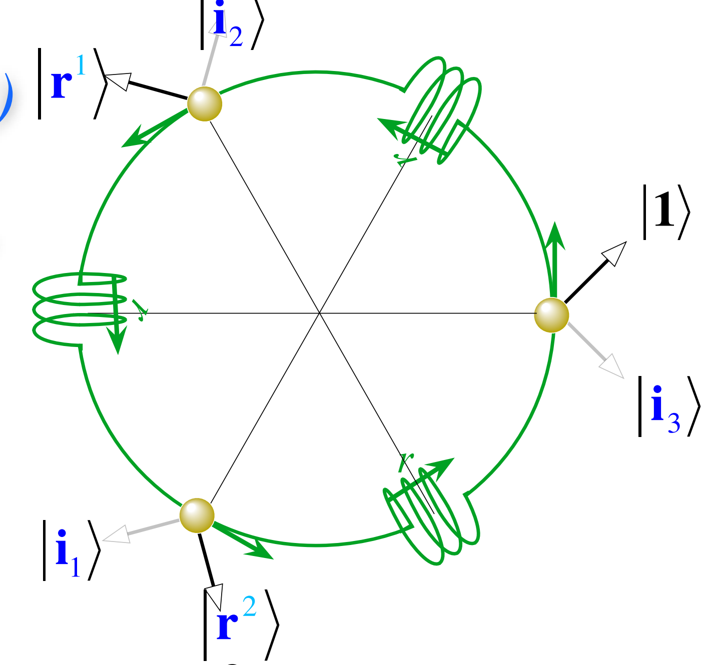
$D_3 \supset C_3(\mathbf{r}^{\pm 1})$ local symmetry K-matrix eigensolutions

Generic K-matrix (Top row)

$$\langle \mathbf{1} | \mathbf{K} | \mathbf{g}_b \rangle = \begin{bmatrix} r_0 & r_1 & r_2 & i_1 & i_2 & i_3 \end{bmatrix}$$

$$\langle \mathbf{1} | \mathbf{K}_{C_3} | \mathbf{g}_b \rangle = \begin{bmatrix} r_0 & ir & -ir & 0 & 0 & 0 \end{bmatrix}$$

$D_3 \supset C_3(\mathbf{r}^{\pm 1})$ local symmetry model



$D_3 \supset C_3(\mathbf{r}^{\pm 1})$ local symmetry vibrational K-matrix

Set: $r_1 = r = -r_2^*$, and: $i_1 = i_2 = i_3 = 0$

$$K_{xx}^{A_1} = r_0 + r_1 + r_1^* + i_1 + i_2 + i_3 = r_0$$

$$K_{yy}^{A_2} = r_0 + r_1 + r_1^* - i_1 - i_2 - i_3 = r_0$$

$$\begin{pmatrix} K_{xx}^{E_1} & K_{xy}^{E_1} \\ K_{yx}^{E_1} & K_{yy}^{E_1} \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 2r_0 - r_1 - r_1^* - i_1 - i_2 + 2i_3 & \sqrt{3}(-r_1 + r_1^* - i_1 + i_2) \\ \sqrt{3}(-r_1^* + r_1 - i_1 + i_2) & 2r_0 - r_1 - r_1^* + i_1 + i_2 - 2i_3 \end{pmatrix}_{\substack{r_1=r=-r_2^* \\ i_1=i_2=i_3=0}} = \begin{pmatrix} r_0 & -ir\frac{\sqrt{3}}{2} \\ +ir\frac{\sqrt{3}}{2} & r_0 \end{pmatrix}$$

$D_3 \supset C_3(\mathbf{r}^{\pm 1})$ local symmetry vibrational K-matrix eigenvalues $K_m/M = \omega_m^2$

$$K_{xx}^{A_1} = r_0$$

$$K_{yy}^{A_2} = r_0$$

$$\begin{pmatrix} K_{xx}^{E_1} & K_{xy}^{E_1} \\ K_{yx}^{E_1} & K_{yy}^{E_1} \end{pmatrix} = \begin{pmatrix} r_0 & -ir\frac{\sqrt{3}}{2} \\ +ir\frac{\sqrt{3}}{2} & r_0 \end{pmatrix} \Rightarrow \begin{pmatrix} r_0 + r\frac{\sqrt{3}}{2} & 0 \\ 0 & r_0 - r\frac{\sqrt{3}}{2} \end{pmatrix}$$

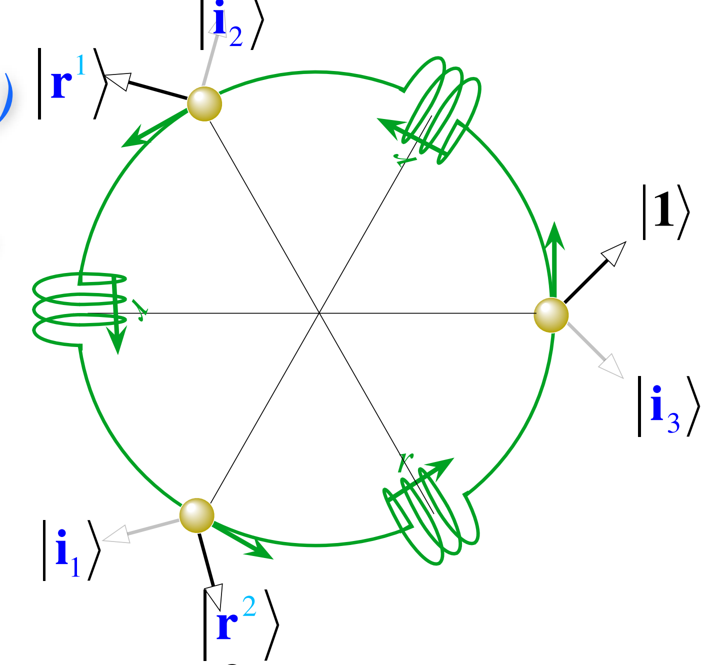
$D_3 \supset C_3(\mathbf{r}^{\pm 1})$ local symmetry K-matrix eigensolutions

Generic K-matrix (Top row)

$$\langle \mathbf{1}|\mathbf{K}|\mathbf{g}_b\rangle = \begin{bmatrix} r_0 & r_1 & r_2 & i_1 & i_2 & i_3 \end{bmatrix}$$

$$\langle \mathbf{1}|\mathbf{K}_{C_3}|\mathbf{g}_b\rangle = \begin{bmatrix} r_0 & ir & -ir & 0 & 0 & 0 \end{bmatrix}$$

$D_3 \supset C_3(\mathbf{r}^{\pm 1})$ local symmetry model



$D_3 \supset C_3(\mathbf{r}^{\pm 1})$ local symmetry vibrational K-matrix

Set: $r_1 = r = -r_2^*$, and: $i_1 = i_2 = i_3 = 0$

$$K_{xx}^{A_1} = r_0 + r_1 + r_1^* + i_1 + i_2 + i_3 = r_0$$

$$K_{yy}^{A_2} = r_0 + r_1 + r_1^* - i_1 - i_2 - i_3 = r_0$$

$$\begin{pmatrix} K_{xx}^{E_1} & K_{xy}^{E_1} \\ K_{yx}^{E_1} & K_{yy}^{E_1} \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 2r_0 - r_1 - r_1^* - i_1 - i_2 + 2i_3 & \sqrt{3}(-r_1 + r_1^* - i_1 + i_2) \\ \sqrt{3}(-r_1^* + r_1 - i_1 + i_2) & 2r_0 - r_1 - r_1^* + i_1 + i_2 - 2i_3 \end{pmatrix}_{\substack{r_1 = r = -r_2^* \\ i_1 = i_2 = i_3 = 0}} = \begin{pmatrix} r_0 & -ir\frac{\sqrt{3}}{2} \\ +ir\frac{\sqrt{3}}{2} & r_0 \end{pmatrix}$$

$D_3 \supset C_3(\mathbf{r}^{\pm 1})$ local symmetry vibrational K-matrix eigenvalues $K_m/M = \omega_m^2$

$$K_{xx}^{A_1} = r_0$$

$$K_{yy}^{A_2} = r_0$$

$$\begin{pmatrix} K_{xx}^{E_1} & K_{xy}^{E_1} \\ K_{yx}^{E_1} & K_{yy}^{E_1} \end{pmatrix} = \begin{pmatrix} r_0 & -ir\frac{\sqrt{3}}{2} \\ +ir\frac{\sqrt{3}}{2} & r_0 \end{pmatrix} \Rightarrow \begin{pmatrix} r_0 + r\frac{\sqrt{3}}{2} & 0 \\ 0 & r_0 - r\frac{\sqrt{3}}{2} \end{pmatrix}$$

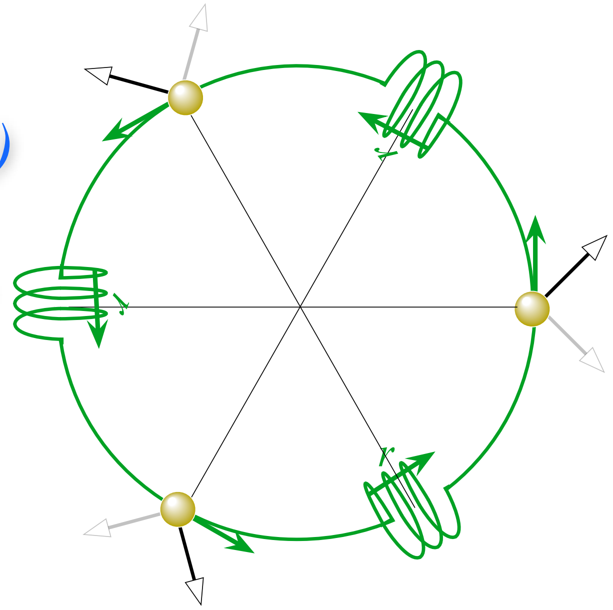
E_1 Eigenvectors in terms of $D_3 \supset C_2(i_3)$ E_1-vectors

$$\mathbf{K}\left|\begin{matrix} E_1 \\ g(1)_3 \end{matrix}\right\rangle = \mathbf{K}\left(\left|\begin{matrix} E_1 \\ gx \end{matrix}\right\rangle + i\left|\begin{matrix} E_1 \\ gy \end{matrix}\right\rangle\right)\frac{1}{\sqrt{2}} = +r\frac{\sqrt{3}}{2}\left|\begin{matrix} E_1 \\ g(1)_3 \end{matrix}\right\rangle,$$

$$\mathbf{K}\left|\begin{matrix} E_1 \\ g(2)_3 \end{matrix}\right\rangle = \mathbf{K}\left(\left|\begin{matrix} E_1 \\ gx \end{matrix}\right\rangle - i\left|\begin{matrix} E_1 \\ gy \end{matrix}\right\rangle\right)\frac{1}{\sqrt{2}} = -r\frac{\sqrt{3}}{2}\left|\begin{matrix} E_1 \\ g(2)_3 \end{matrix}\right\rangle.$$

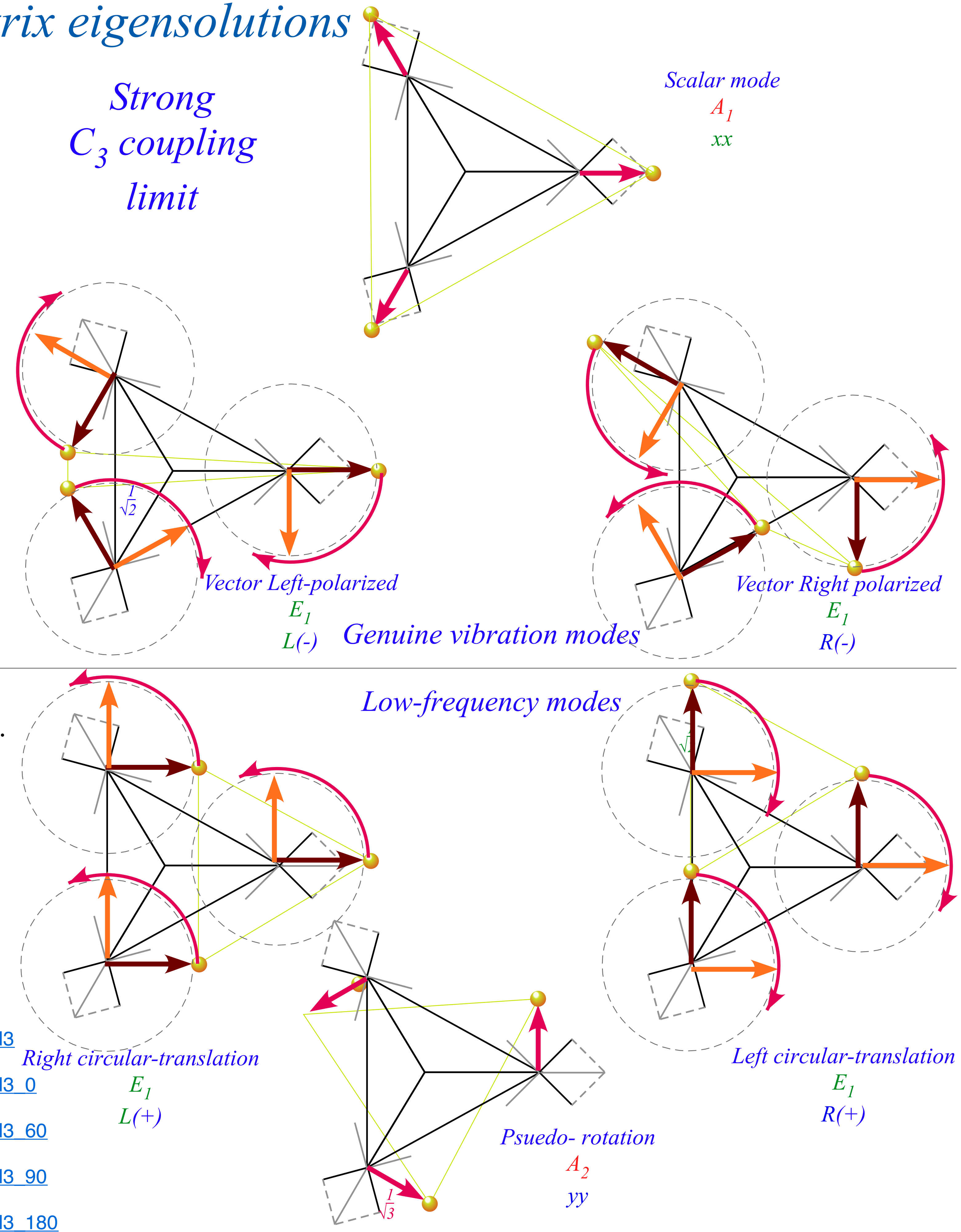
$D_3 \supset C_3(\mathbf{r}^{\pm 1})$ local symmetry K-matrix eigensolutions

$D_3 \supset C_3(\mathbf{r}^{\pm 1})$ local symmetry model



$$\mathbf{K}\left|\begin{matrix}E_1\\ g(1)_3\end{matrix}\right\rangle = \mathbf{K}\left(\left|\begin{matrix}E_1\\ gx\end{matrix}\right\rangle + i\left|\begin{matrix}E_1\\ gy\end{matrix}\right\rangle\right)\frac{1}{\sqrt{2}} = +r\sqrt{\tfrac{3}{2}}\left|\begin{matrix}E_1\\ g(1)_3\end{matrix}\right\rangle,$$

$$\mathbf{K}\left|\begin{matrix}E_1\\ g(2)_3\end{matrix}\right\rangle = \mathbf{K}\left(\left|\begin{matrix}E_1\\ gx\end{matrix}\right\rangle - i\left|\begin{matrix}E_1\\ gy\end{matrix}\right\rangle\right)\frac{1}{\sqrt{2}} = -r\sqrt{\tfrac{3}{2}}\left|\begin{matrix}E_1\\ g(2)_3\end{matrix}\right\rangle.$$



https://modphys.hosted.uark.edu/markup/MolVibesWeb.html?scenario=C3vN3

https://modphys.hosted.uark.edu/markup/MolVibesWeb.html?scenario=C3vN3_0

https://modphys.hosted.uark.edu/markup/MolVibesWeb.html?scenario=C3vN3_60

https://modphys.hosted.uark.edu/markup/MolVibesWeb.html?scenario=C3vN3_90

https://modphys.hosted.uark.edu/markup/MolVibesWeb.html?scenario=C3vN3_180

AMOP reference links on page 2

2.26.18 class 14.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

Discrete symmetry subgroups of O(3) using Mock-Mach principle: $D_3 \sim C_{3v}$ LAB vs BOD
Vibrational eigensolutions, $D_6 \sim C_{6v}$ bands, subgroup correlation, and Frobenius reciprocity

Review: *H-matrix Global vs Local symmetry*

Molecular vibration K-matrix symmetry analogous to quantum H-matrix

Molecular K-matrix construction

$D_3 \supset C_2(i_3)$ local-symmetry K-matrix eigensolutions

D_3-direct-connection K-matrix eigenstates mix local symmetry

$D_3 \supset C_3(\mathbf{r}^{\pm 1})$ moving-wave local symmetry K-matrix "Coriolis" eigensolutions

Applied symmetry reduction and splitting

Subduced irep $D^\alpha(D^3)\downarrow C_2 = d^{0_2} \oplus d^{1_2} \oplus ..$ correlation

Subduced irep $D^\alpha(D^3)\downarrow C_3 = d^{0_3} \oplus d^{1_3} \oplus ..$ correlation

Spontaneous symmetry breaking and clustering: Frobenius Reciprocity and band structure

Induced rep $d^a(C_2)\uparrow D^3 = D^\alpha \oplus D^\beta \oplus ..$ correlation

Induced rep $d^a(C_3)\uparrow D^3 = D^\alpha \oplus D^\beta \oplus ..$ correlation

D_6 symmetry and Hexagonal Bands

Cross product of the C_2 and D_3 characters gives all $D_6 = D_3 \times C_2$ characters and ireps

D_6 Band structure and related Global vs Local induced representations, *D_4 example*

U(12)-Supersymmetry

Applied symmetry reduction and splitting:
Subduced irep $D^{\alpha}(D^{3})\downarrow C_2 = d^{0_2} \oplus d^{1_2} \oplus ..$ *correlation*

$D_3 \supset C_2$	0_2	1_2
A_1	1	·
A_2	·	1
E_1	1	1

$\chi_k^{\alpha}(D_3)$	$\chi_{\mathbf{1}}^{\alpha}$	$\chi_{\mathbf{r}^{1,2}}^{\alpha}$	$\chi_{\mathbf{i}_{1,2,3}}^{\alpha}$
$\alpha = A_1$	1	1	1
$\alpha = A_2$	1	1	-1
$\alpha = E$	2	-1	0

$\chi_k^{\alpha}(C_2)$	$\chi_{\mathbf{1}}^{\alpha}$	$\chi_{\mathbf{i}_3}^{\alpha}$
$\alpha = 0_2$	1	1
$\alpha = 1_2$	1	-1

Applied symmetry reduction and splitting:
Subduced irep $D^{\alpha}(D^3)\downarrow C_2 = d^{0_2} \oplus d^{1_2} \oplus$.. correlation

$D_3 \supset C_2$	$\mathbf{P}^{\alpha}$ *relabel/split*	D^{α} *relabel/reduce*	ω^{α} *relabel/split*
A_1	$\mathbf{P}^{A_1} = \mathbf{P}^{A_1}\mathbf{P}^{0_2} = \mathbf{P}^{A_1}_{0_2 0_2}$	$\Rightarrow D^{A_1}\downarrow C_2 \sim d^{0_2}$	$\Rightarrow \omega^{A_1} \to \omega^{0_2}$
A_2	$\mathbf{P}^{A_2} = \mathbf{P}^{A_2}\mathbf{P}^{1_2} = \mathbf{P}^{A_2}_{1_2 1_2}$	$\Rightarrow D^{A_2}\downarrow C_2 \sim d^{1_2}$	$\Rightarrow \omega^{A_2} \to \omega^{1_2}$
E_1	$\mathbf{P}^{E_1} = \mathbf{P}^{E_1}\mathbf{P}^{0_2} + \mathbf{P}^{E_1}\mathbf{P}^{1_2}$ $= \mathbf{P}^{E_1}_{0_2 0_2} + \mathbf{P}^{E_1}_{1_2 1_2}$	$\Rightarrow D^{E_1}\downarrow C_2 \sim$ $d^{0_2} \oplus d^{1_2}$	$\Rightarrow \omega^{E_1} \to \omega^{0_2}$ $\searrow \omega^{1_2}$

$D_3 \supset C_2$	0_2	1_2
A_1	1	·
A_2	·	1
E_1	1	1

$\chi^{\alpha}_k(D_3)$	$\chi^{\alpha}_{\mathbf{1}}$	$\chi^{\alpha}_{\mathbf{r}^{1,2}}$	$\chi^{\alpha}_{\mathbf{i}_{1,2,3}}$
$\alpha = A_1$	1	1	1
$\alpha = A_2$	1	1	-1
$\alpha = E$	2	-1	0

$\chi^{\alpha}_k(C_2)$	$\chi^{\alpha}_{\mathbf{1}}$	$\chi^{\alpha}_{\mathbf{i}_3}$
$\alpha = 0_2$	1	1
$\alpha = 1_2$	1	-1

Key concept:
P*rojector splitting*
means
Level splitting
Level

Applied symmetry reduction and splitting:

Subduced irep $D^{\alpha}(D^3)\downarrow C_2 = d^{0_2} \oplus d^{1_2} \oplus ..$ *correlation*

$D_3 \supset C_2$	$\mathbf{P}^{\alpha}$ *relabel/split*	D^{α} *relabel/reduce*	ω^{α} *relabel/split*
A_1	$\mathbf{P}^{A_1} = \mathbf{P}^{A_1}\mathbf{P}^{0_2} = \mathbf{P}^{A_1}_{0_2 0_2}$	$\Rightarrow D^{A_1}\downarrow C_2 \sim d^{0_2}$	$\Rightarrow \omega^{A_1} \rightarrow \omega^{0_2}$
A_2	$\mathbf{P}^{A_2} = \mathbf{P}^{A_2}\mathbf{P}^{1_2} = \mathbf{P}^{A_2}_{1_2 1_2}$	$\Rightarrow D^{A_2}\downarrow C_2 \sim d^{1_2}$	$\Rightarrow \omega^{A_2} \rightarrow \omega^{1_2}$
E_1	$\mathbf{P}^{E_1} = \mathbf{P}^{E_1}\mathbf{P}^{0_2} + \mathbf{P}^{E_1}\mathbf{P}^{1_2} = \mathbf{P}^{E_1}_{0_2 0_2} + \mathbf{P}^{E_1}_{1_2 1_2}$	$\Rightarrow D^{E_1}\downarrow C_2 \sim d^{0_2} \oplus d^{1_2}$	$\Rightarrow \omega^{E_1} \rightarrow \omega^{0_2}$, $\searrow \omega^{1_2}$

$D_3 \supset C_2$	0_2	1_2
A_1	1	·
A_2	·	1
E_1	1	1

Key concept:

P*rojector splitting*

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$\chi^{\alpha}_k(D_3)$	$\chi^{\alpha}_{\mathbf{1}}$	$\chi^{\alpha}_{\mathbf{r}^{1,2}}$	$\chi^{\alpha}_{\mathbf{i}_{1,2,3}}$
$\alpha = A_1$	1	1	1
$\alpha = A_2$	1	1	−1
$\alpha = E$	2	−1	0

$\chi^{\alpha}_k(C_2)$	$\chi^{\alpha}_{\mathbf{1}}$	$\chi^{\alpha}_{\mathbf{i}_1}$
$\alpha = 0_2$	1	1
$\alpha = 1_2$	1	−1

$\chi^{\alpha}_k(C_3)$	$\chi^{\alpha}_{\mathbf{1}}$	$\chi^{\alpha}_{\mathbf{r}^1}$	$\chi^{\alpha}_{\mathbf{r}^2}$
$\alpha = 0_3$	1	1	1
$\alpha = 1_3$	1	$e^{-i\frac{2\pi}{3}}$	$e^{i\frac{2\pi}{3}}$
$\alpha = 2_3$	1	$e^{i\frac{2\pi}{3}}$	$e^{-i\frac{2\pi}{3}}$

Applied symmetry reduction and splitting:

Subduced irep $D^{\alpha}(D^3)\downarrow C_3 = d^{03} \oplus d^{13} \oplus ..$ *correlation*

Applied symmetry reduction and splitting:
Subduced irep $D^{\alpha}(D^3)\downarrow C_2 = d^{0_2} \oplus d^{1_2} \oplus$.. correlation

$D_3 \supset C_2$	$\mathbf{P}^{\alpha}$ *relabel/split*	D^{α} *relabel/reduce*	ω^{α} *relabel/split*
A_1	$\mathbf{P}^{A_1} = \mathbf{P}^{A_1}\mathbf{P}^{0_2} = \mathbf{P}^{A_1}_{0_2 0_2}$	$\Rightarrow D^{A_1}\downarrow C_2 \sim d^{0_2}$	$\Rightarrow \omega^{A_1} \rightarrow \omega^{0_2}$
A_2	$\mathbf{P}^{A_2} = \mathbf{P}^{A_2}\mathbf{P}^{1_2} = \mathbf{P}^{A_2}_{1_2 1_2}$	$\Rightarrow D^{A_2}\downarrow C_2 \sim d^{1_2}$	$\Rightarrow \omega^{A_2} \rightarrow \omega^{1_2}$
E_1	$\mathbf{P}^{E_1} = \mathbf{P}^{E_1}\mathbf{P}^{0_2} + \mathbf{P}^{E_1}\mathbf{P}^{1_2}$	$\Rightarrow D^{E_1}\downarrow C_2 \sim$	$\Rightarrow \omega^{E_1} \rightarrow \omega^{0_2}$
	$= \mathbf{P}^{E_1}_{0_2 0_2} + \mathbf{P}^{E_1}_{1_2 1_2}$	$d^{0_2} \oplus d^{1_2}$	$\searrow \omega^{1_2}$

$D_3 \supset C_2$	0_2	1_2
A_1	1	·
A_2	·	1
E_1	1	1

$\chi^{\alpha}_k(D_3)$	$\chi^{\alpha}_{\mathbf{1}}$	$\chi^{\alpha}_{\mathbf{r}^{1,2}}$	$\chi^{\alpha}_{\mathbf{i}_{1,2,3}}$
$\alpha = A_1$	1	1	1
$\alpha = A_2$	1	1	−1
$\alpha = E$	2	−1	0

$\chi^{\alpha}_k(C_2)$	$\chi^{\alpha}_{\mathbf{1}}$	$\chi^{\alpha}_{\mathbf{i}}$
$\alpha = 0_2$	1	1
$\alpha = 1_2$	1	−1

$\chi^{\alpha}_k(C_3)$	$\chi^{\alpha}_{\mathbf{1}}$	$\chi^{\alpha}_{\mathbf{r}^1}$	$\chi^{\alpha}_{\mathbf{r}^2}$
$\alpha = 0_3$	1	1	1
$\alpha = 1_3$	1	$e^{-i\frac{2\pi}{3}}$	$e^{i\frac{2\pi}{3}}$
$\alpha = 2_3$	1	$e^{i\frac{2\pi}{3}}$	$e^{-i\frac{2\pi}{3}}$

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Applied symmetry reduction and splitting:
Subduced irep $D^{\alpha}(D^3)\downarrow C_3 = d^{03} \oplus d^{13} \oplus$.. correlation

$D_3 \supset C_3$	$\mathbf{P}^{\alpha}$ *relabel/split*	D^{α} *relabel/reduce*	ω^{α} *relabel/split*
A_1	$\mathbf{P}^{A_1} = \mathbf{P}^{A_1}\mathbf{P}^{0_3} = \mathbf{P}^{A_1}_{0_3 0_3}$	$\Rightarrow D^{A_1}\downarrow C_3 \sim d^{0_3}$	$\Rightarrow \omega^{A_1} \rightarrow \omega^{0_3}$
A_2	$\mathbf{P}^{A_2} = \mathbf{P}^{A_2}\mathbf{P}^{0_3} = \mathbf{P}^{A_2}_{0_3 0_3}$	$\Rightarrow D^{A_2}\downarrow C_3 \sim d^{0_3}$	$\Rightarrow \omega^{A_2} \rightarrow \omega^{0_3}$
E_1	$\mathbf{P}^{E_1} = \mathbf{P}^{E_1}\mathbf{P}^{1_3} + \mathbf{P}^{E_1}\mathbf{P}^{2_3}$	$\Rightarrow D^{E_1}\downarrow C_3 \sim$	$\Rightarrow \omega^{E_1} \rightarrow \omega^{1_3}$
	$= \mathbf{P}^{E_1}_{1_3 1_3} + \mathbf{P}^{E_1}_{2_3 2_3}$	$d^{1_3} \oplus d^{2_3}$	$\searrow \omega^{2_3}$

$D_3 \supset C_3$	0_3	1_3	2_3
A_1	1	·	·
A_2	1	·	·
E_1	·	1	1

Applied symmetry reduction and splitting:
Subduced irep $D^{\alpha}(D^3)\downarrow C_2 = d^{0_2} \oplus d^{1_2} \oplus$.. correlation

$D_3 \supset C_2$	$\mathbf{P}^{\alpha}$ *relabel/split*	D^{α} *relabel/reduce*	ω^{α} *relabel/split*
A_1	$\mathbf{P}^{A_1} = \mathbf{P}^{A_1}\mathbf{P}^{0_2} = \mathbf{P}^{A_1}_{0_2 0_2}$	$\Rightarrow D^{A_1}\downarrow C_2 \sim d^{0_2}$	$\Rightarrow \omega^{A_1} \rightarrow \omega^{0_2}$
A_2	$\mathbf{P}^{A_2} = \mathbf{P}^{A_2}\mathbf{P}^{1_2} = \mathbf{P}^{A_2}_{1_2 1_2}$	$\Rightarrow D^{A_2}\downarrow C_2 \sim d^{1_2}$	$\Rightarrow \omega^{A_2} \rightarrow \omega^{1_2}$
E_1	$\mathbf{P}^{E_1} = \mathbf{P}^{E_1}\mathbf{P}^{0_2} + \mathbf{P}^{E_1}\mathbf{P}^{1_2}$	$\Rightarrow D^{E_1}\downarrow C_2 \sim$	$\Rightarrow \omega^{E_1} \rightarrow \omega^{0_2}$
	$= \mathbf{P}^{E_1}_{0_2 0_2} + \mathbf{P}^{E_1}_{1_2 1_2}$	$d^{0_2} \oplus d^{1_2}$	$\searrow \omega^{1_2}$

$D_3 \supset C_2$	0_2	1_2	
A_1	1	·	$D^{A_1}(D_3)\downarrow C_2 \sim d^{0_2}$
A_2	·	1	$D^{A_2}(D_3)\downarrow C_2 \sim d^{1_2}$
E_1	1	1	$D^{E_1}(D_3)\downarrow C_2 \sim d^{0_2} \oplus d^{1_2}$

$\chi^{\alpha}_k(D_3)$	$\chi^{\alpha}_{\mathbf{1}}$	$\chi^{\alpha}_{\mathbf{r}^{1,2}}$	$\chi^{\alpha}_{\mathbf{i}_{1,2,3}}$
$\alpha = A_1$	1	1	1
$\alpha = A_2$	1	1	-1
$\alpha = E$	2	-1	0

$\chi^{\alpha}_k(C_2)$	$\chi^{\alpha}_{\mathbf{1}}$	$\chi^{\alpha}_{\mathbf{i}}$
$\alpha = 0_2$	1	1
$\alpha = 1_2$	1	-1

$\chi^{\alpha}_k(C_3)$	$\chi^{\alpha}_{\mathbf{1}}$	$\chi^{\alpha}_{\mathbf{r}^1}$	$\chi^{\alpha}_{\mathbf{r}^2}$
$\alpha = 0_3$	1	1	1
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E_1	$\mathbf{P}^{E_1} = \mathbf{P}^{E_1}\mathbf{P}^{1_3} + \mathbf{P}^{E_1}\mathbf{P}^{2_3}$	$\Rightarrow D^{E_1}\downarrow C_3 \sim$	$\Rightarrow \omega^{E_1} \rightarrow \omega^{1_3}$
	$= \mathbf{P}^{E_1}_{1_3 1_3} + \mathbf{P}^{E_1}_{2_3 2_3}$	$d^{1_3} \oplus d^{2_3}$	$\searrow \omega^{2_3}$

$D_3 \supset C_3$	0_3	1_3	2_3	
A_1	1	·	·	$D^{A_1}(D_3)\downarrow C_3 \sim d^{0_3}$
A_2	1	·	·	$D^{A_2}(D_3)\downarrow C_3 \sim d^{0_3}$
E_1	·	1	1	$D^{E_1}(D_3)\downarrow C_3 \sim d^{1_3} \oplus d^{2_3}$

AMOP reference links on page 2

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William G. Harter - University of Arkansas

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Induced rep $d^{a}(C_2) \uparrow D^3 = D^{\alpha} \oplus D^{\beta} \oplus ..$ correlation

Induced rep $d^{a}(C_3) \uparrow D^3 = D^{\alpha} \oplus D^{\beta} \oplus ..$ correlation

D_6 symmetry and Hexagonal Bands

Cross product of the C_2 and D_3 characters gives all $D_6 = D_3 \times C_2$ characters and ireps

D_6 Band structure and related Global vs Local induced representations, D_4 example

U(12)-Supersymmetry

Applied symmetry reduction and splitting:
Subduced irep $D^{\alpha}(D^3)\downarrow C_2 = d^{0_2} \oplus d^{1_2} \oplus ..$ correlation

$D_3 \supset C_2$	$\mathbf{P}^{\alpha}$ *relabel/split*	D^{α} *relabel/reduce*	ω^{α} *relabel/split*
A_1	$\mathbf{P}^{A_1}=\mathbf{P}^{A_1}\mathbf{P}^{0_2}=\mathbf{P}^{A_1}_{0_2 0_2}$	$\Rightarrow D^{A_1}\downarrow C_2 \sim d^{0_2}$	$\Rightarrow \omega^{A_1} \rightarrow \omega^{0_2}$
A_2	$\mathbf{P}^{A_2}=\mathbf{P}^{A_2}\mathbf{P}^{1_2}=\mathbf{P}^{A_2}_{1_2 1_2}$	$\Rightarrow D^{A_2}\downarrow C_2 \sim d^{1_2}$	$\Rightarrow \omega^{A_2} \rightarrow \omega^{1_2}$
E_1	$\mathbf{P}^{E_1}=\mathbf{P}^{E_1}\mathbf{P}^{0_2}+\mathbf{P}^{E_1}\mathbf{P}^{1_2}$	$\Rightarrow D^{E_1}\downarrow C_2 \sim$	$\Rightarrow \omega^{E_1} \rightarrow \omega^{0_2}$
	$=\mathbf{P}^{E_1}_{0_2 0_2}+\mathbf{P}^{E_1}_{1_2 1_2}$	$d^{0_2} \oplus d^{1_2}$	$\searrow \omega^{1_2}$

$D_3 \supset C_2$	0_2	1_2	
A_1	1	·	$D^{A_1}(D_3)\downarrow C_2 \sim d^{0_2}$
A_2	·	1	$D^{A_2}(D_3)\downarrow C_2 \sim d^{1_2}$
E_1	1	1	$D^{E_1}(D_3)\downarrow C_2 \sim d^{0_2} \oplus d^{1_2}$

Applied symmetry reduction and splitting:
Subduced irep $D^{\alpha}(D^3)\downarrow C_3 = d^{03} \oplus d^{13} \oplus ..$ correlation

$D_3 \supset C_3$	$\mathbf{P}^{\alpha}$ *relabel/split*	D^{α} *relabel/reduce*	ω^{α} *relabel/split*
A_1	$\mathbf{P}^{A_1}=\mathbf{P}^{A_1}\mathbf{P}^{0_3}=\mathbf{P}^{A_1}_{0_3 0_3}$	$\Rightarrow D^{A_1}\downarrow C_3 \sim d^{0_3}$	$\Rightarrow \omega^{A_1} \rightarrow \omega^{0_3}$
A_2	$\mathbf{P}^{A_2}=\mathbf{P}^{A_2}\mathbf{P}^{0_3}=\mathbf{P}^{A_2}_{0_3 0_3}$	$\Rightarrow D^{A_2}\downarrow C_3 \sim d^{0_3}$	$\Rightarrow \omega^{A_2} \rightarrow \omega^{0_3}$
E_1	$\mathbf{P}^{E_1}=\mathbf{P}^{E_1}\mathbf{P}^{1_3}+\mathbf{P}^{E_1}\mathbf{P}^{2_3}$	$\Rightarrow D^{E_1}\downarrow C_3 \sim$	$\Rightarrow \omega^{E_1} \rightarrow \omega^{1_3}$
	$=\mathbf{P}^{E_1}_{1_3 1_3}+\mathbf{P}^{E_1}_{2_3 2_3}$	$d^{1_3} \oplus d^{2_3}$	$\searrow \omega^{2_3}$

$D_3 \supset C_3$	0_3	1_3	2_3	
A_1	1	·	·	$D^{A_1}(D_3)\downarrow C_3 \sim d^{0_3}$
A_2	1	·	·	$D^{A_2}(D_3)\downarrow C_3 \sim d^{0_3}$
E_1	·	1	1	$D^{E_1}(D_3)\downarrow C_3 \sim d^{1_3} \oplus d^{2_3}$

Applied symmetry reduction and splitting:
Subduced irep $D^{\alpha}(D^3)\downarrow C_2 = d^{0_2}\oplus d^{1_2}\oplus$.. correlation

$D_3 \supset C_2$	$\mathbf{P}^{\alpha}$ relabel/split	D^{α} relabel/reduce	ω^{α} relabel/split
A_1	$\mathbf{P}^{A_1}=\mathbf{P}^{A_1}\mathbf{P}^{0_2}=\mathbf{P}^{A_1}_{0_2 0_2}$	$\Rightarrow D^{A_1}\downarrow C_2 \sim d^{0_2}$	$\Rightarrow \omega^{A_1}\rightarrow \omega^{0_2}$
A_2	$\mathbf{P}^{A_2}=\mathbf{P}^{A_2}\mathbf{P}^{1_2}=\mathbf{P}^{A_2}_{1_2 1_2}$	$\Rightarrow D^{A_2}\downarrow C_2 \sim d^{1_2}$	$\Rightarrow \omega^{A_2}\rightarrow \omega^{1_2}$
E_1	$\mathbf{P}^{E_1}=\mathbf{P}^{E_1}\mathbf{P}^{0_2}+\mathbf{P}^{E_1}\mathbf{P}^{1_2}$	$\Rightarrow D^{E_1}\downarrow C_2 \sim$	$\Rightarrow \omega^{E_1}\rightarrow \omega^{0_2}$
	$=\mathbf{P}^{E_1}_{0_2 0_2}+\mathbf{P}^{E_1}_{1_2 1_2}$	$d^{0_2}\oplus d^{1_2}$	$\searrow \omega^{1_2}$

$D_3 \supset C_2$	0_2	1_2	
A_1	1	·	$D^{A_1}(D_3)\downarrow C_2 \sim d^{0_2}$
A_2	·	1	$D^{A_2}(D_3)\downarrow C_2 \sim d^{1_2}$
E_1	1	1	$D^{E_1}(D_3)\downarrow C_2 \sim d^{0_2}\oplus d^{1_2}$

$d^{0_2}(C_2)\Uparrow D_3 \sim D^{A_1}\oplus D^{E_1}$

$d^{1_2}(C_2)\Uparrow D_3 \sim D^{A_2}\oplus D^{E_1}$

Spontaneous symmetry breaking and clustering:
Induced rep $d^a(C_2)\uparrow D^3 = D^{\alpha}\oplus D^{\beta}\oplus$.. correlation

Applied symmetry reduction and splitting:
Subduced irep $D^{\alpha}(D^3)\downarrow C_3 = d^{03}\oplus d^{13}\oplus$.. correlation

$D_3 \supset C_3$	$\mathbf{P}^{\alpha}$ relabel/split	D^{α} relabel/reduce	ω^{α} relabel/split
A_1	$\mathbf{P}^{A_1}=\mathbf{P}^{A_1}\mathbf{P}^{0_3}=\mathbf{P}^{A_1}_{0_3 0_3}$	$\Rightarrow D^{A_1}\downarrow C_3 \sim d^{0_3}$	$\Rightarrow \omega^{A_1}\rightarrow \omega^{0_3}$
A_2	$\mathbf{P}^{A_2}=\mathbf{P}^{A_2}\mathbf{P}^{0_3}=\mathbf{P}^{A_2}_{0_3 0_3}$	$\Rightarrow D^{A_2}\downarrow C_3 \sim d^{0_3}$	$\Rightarrow \omega^{A_2}\rightarrow \omega^{0_3}$
E_1	$\mathbf{P}^{E_1}=\mathbf{P}^{E_1}\mathbf{P}^{1_3}+\mathbf{P}^{E_1}\mathbf{P}^{2_3}$	$\Rightarrow D^{E_1}\downarrow C_3 \sim$	$\Rightarrow \omega^{E_1}\rightarrow \omega^{1_3}$
	$=\mathbf{P}^{E_1}_{1_3 1_3}+\mathbf{P}^{E_1}_{2_3 2_3}$	$d^{1_3}\oplus d^{2_3}$	$\searrow \omega^{2_3}$

$D_3 \supset C_3$	0_3	1_3	2_3	
A_1	1	·	·	$D^{A_1}(D_3)\downarrow C_3 \sim d^{0_3}$
A_2	1	·	·	$D^{A_2}(D_3)\downarrow C_3 \sim d^{0_3}$
E_1	·	1	1	$D^{E_1}(D_3)\downarrow C_3 \sim d^{1_3}\oplus d^{2_3}$

Applied symmetry reduction and splitting:
Subduced irep $D^{\alpha}(D^3)\downarrow C_2 = d^{0_2} \oplus d^{1_2} \oplus$.. correlation

$D_3 \supset C_2$	$\mathbf{P}^{\alpha}$ *relabel/split*	D^{α} *relabel/reduce*	ω^{α} *relabel/split*
A_1	$\mathbf{P}^{A_1}=\mathbf{P}^{A_1}\mathbf{P}^{0_2}=\mathbf{P}^{A_1}_{0_2 0_2}$	$\Rightarrow D^{A_1}\downarrow C_2 \sim d^{0_2}$	$\Rightarrow \omega^{A_1} \rightarrow \omega^{0_2}$
A_2	$\mathbf{P}^{A_2}=\mathbf{P}^{A_2}\mathbf{P}^{1_2}=\mathbf{P}^{A_2}_{1_2 1_2}$	$\Rightarrow D^{A_2}\downarrow C_2 \sim d^{1_2}$	$\Rightarrow \omega^{A_2} \rightarrow \omega^{1_2}$
E_1	$\mathbf{P}^{E_1}=\mathbf{P}^{E_1}\mathbf{P}^{0_2}+\mathbf{P}^{E_1}\mathbf{P}^{1_2} = \mathbf{P}^{E_1}_{0_2 0_2}+\mathbf{P}^{E_1}_{1_2 1_2}$	$\Rightarrow D^{E_1}\downarrow C_2 \sim d^{0_2}\oplus d^{1_2}$	$\Rightarrow \omega^{E_1} \rightarrow \omega^{0_2}$, $\searrow \omega^{1_2}$

$D_3 \supset C_2$	0_2	1_2	
A_1	1	·	$D^{A_1}(D_3)\downarrow C_2 \sim d^{0_2}$
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E_1	1	1	$D^{E_1}(D_3)\downarrow C_2 \sim d^{0_2}\oplus d^{1_2}$

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$D_3 \supset C_3$	$\mathbf{P}^{\alpha}$ *relabel/split*	D^{α} *relabel/reduce*	ω^{α} *relabel/split*
A_1	$\mathbf{P}^{A_1}=\mathbf{P}^{A_1}\mathbf{P}^{0_3}=\mathbf{P}^{A_1}_{0_3 0_3}$	$\Rightarrow D^{A_1}\downarrow C_3 \sim d^{0_3}$	$\Rightarrow \omega^{A_1} \rightarrow \omega^{0_3}$
A_2	$\mathbf{P}^{A_2}=\mathbf{P}^{A_2}\mathbf{P}^{0_3}=\mathbf{P}^{A_2}_{0_3 0_3}$	$\Rightarrow D^{A_2}\downarrow C_3 \sim d^{0_3}$	$\Rightarrow \omega^{A_2} \rightarrow \omega^{0_3}$
E_1	$\mathbf{P}^{E_1}=\mathbf{P}^{E_1}\mathbf{P}^{1_3}+\mathbf{P}^{E_1}\mathbf{P}^{2_3} = \mathbf{P}^{E_1}_{1_3 1_3}+\mathbf{P}^{E_1}_{2_3 2_3}$	$\Rightarrow D^{E_1}\downarrow C_3 \sim d^{1_3}\oplus d^{2_3}$	$\Rightarrow \omega^{E_1} \rightarrow \omega^{1_3}$, $\searrow \omega^{2_3}$

$D_3 \supset C_3$	0_3	1_3	2_3	
A_1	1	·	·	$D^{A_1}(D_3)\downarrow C_3 \sim d^{0_3}$
A_2	1	·	·	$D^{A_2}(D_3)\downarrow C_3 \sim d^{0_3}$
E_1	·	1	1	$D^{E_1}(D_3)\downarrow C_3 \sim d^{1_3}\oplus d^{2}$

$d^{0_3}(C_3)\Uparrow D_3 \sim D^{A_1}\oplus D^{A_2}$

$d^{1_3}(C_3)\Uparrow D_3 \sim D^{E_1}$

$d^{2_3}(C_3)\Uparrow D_3 \sim D^{E_1}$

Spontaneous symmetry breaking and clustering:
Induced rep $d^{a}(C_3)\uparrow D^3 = D^{\alpha}\oplus D^{\beta}\oplus$.. correlation

Frobenius Reciprocity Theorem

Number of $D^{\alpha}(G)$ in $d^{k}(K)\uparrow G =$ Number of $d^{k}(K)$ in $D^{\alpha}(G)\downarrow K$

Frobenius Reciprocity Theorem

Number of $D^{\alpha}(G)$ in $d^{k}(K)\uparrow G =$ Number of $d^{k}(K)$ in $D^{\alpha}(G)\downarrow K$

..and regular representation

$D_3 \supset C_1$	$0_1 = 1_1$
A_1	1
A_2	1
E_1	2

Frobenius Reciprocity Theorem

Number of $D^{\alpha}(G)$ in $d^{k}(K)\uparrow G =$ Number of $d^{k}(K)$ in $D^{\alpha}(G)\downarrow K$

..and regular representation

$D_3 \supset C_1$	$0_1 = 1_1$
A_1	1
A_2	1
E_1	2

$D_3 \supset C_2$	0_2	1_2
A_1	1	·
A_2	·	1
E_1	1	1

$D_3 \supset C_3$	0_3	1_3	2_3
A_1	1	·	·
A_2	1	·	·
E_1	·	1	1

AMOP reference links on page 2

2.26.18 class 14.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

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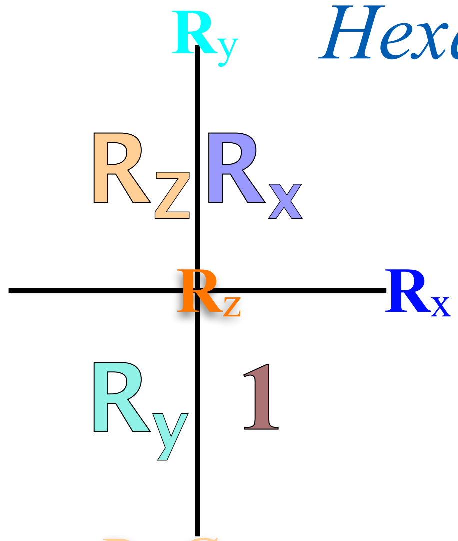
D_6 symmetry and Hexagonal Bands

Cross product of the C_2 and D_3 characters gives all $D_6 = D_3 \times C_2$ characters and ireps

D_6 Band structure and related Global vs Local induced representations, *D_4 example*

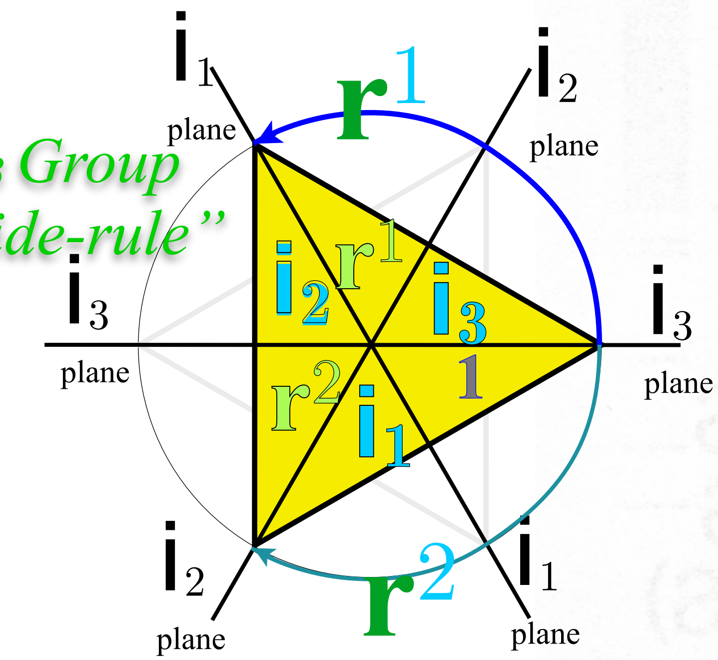
U(12)-Supersymmetry

Hexagonal chains: $D_6 \supset D_3 \supset C_2$ or $D_{6h} \supset D_{2h} \supset D_2$ label 6-fold bands

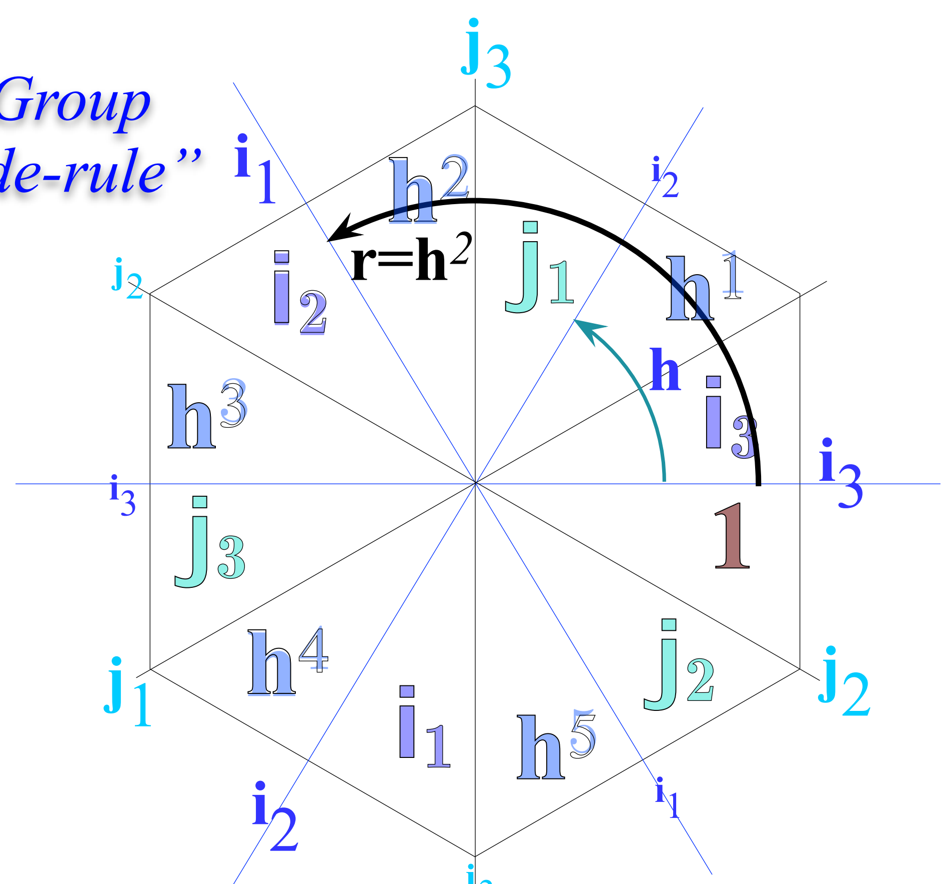


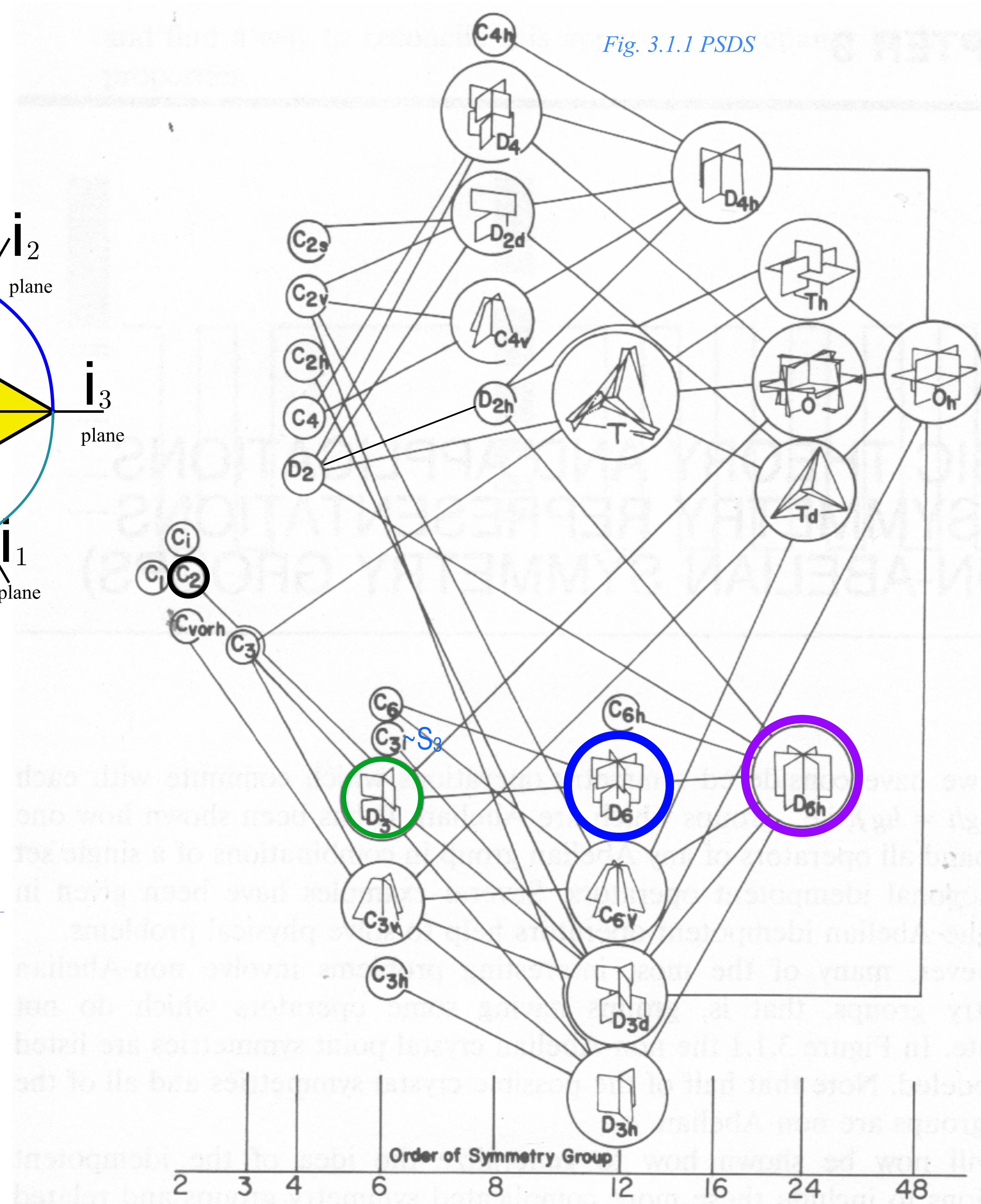
D_2 Group "slide-rule"

D_3 Group "slide-rule"



D_6Group "slide-rule"





Hexagonal chains: $D_6 \supset D_3 \supset C_2$ or $D_{6h} \supset D_{2h} \supset D_2$ label 6-fold bands

D_6 is the *outer product* ($\times$) *product* $D_3 \times C_2$ of D_3 and C_2. (Requires C_2 to commute with all of D_3.)

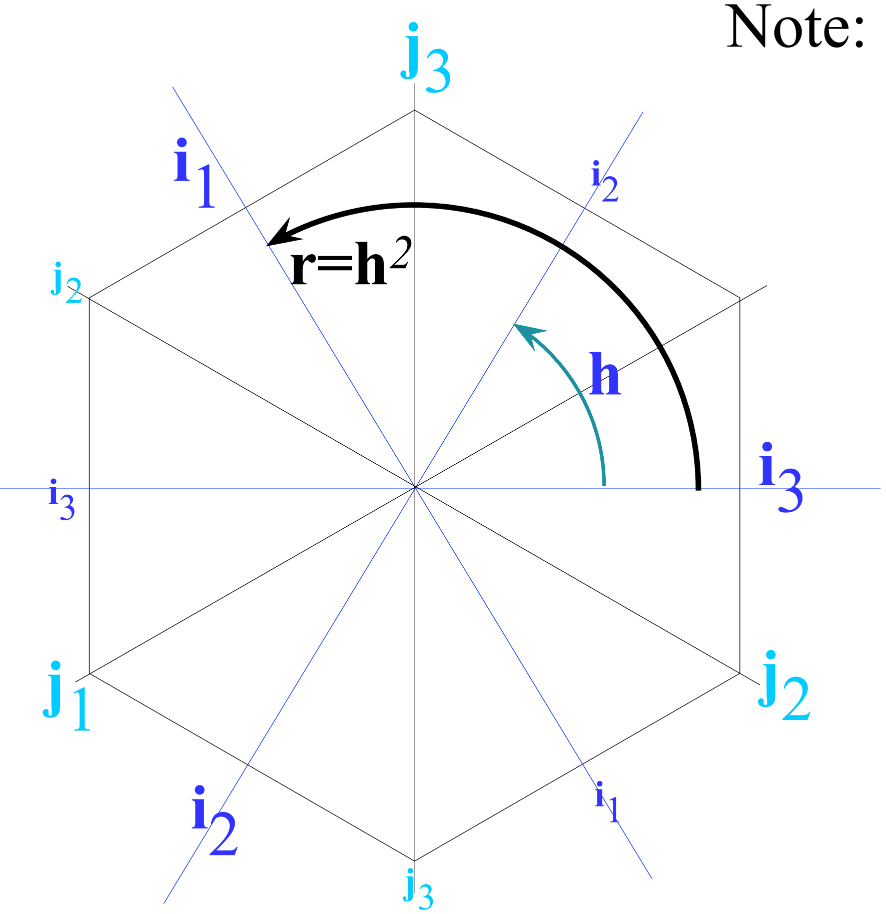
$$D_6 = D_3 \times C_2 = \{\mathbf{1}, \mathbf{r}, \mathbf{r}^2, \mathbf{i}_1, \mathbf{i}_2, \mathbf{i}_3\} \times \{\mathbf{1}, \mathbf{R}_z\}$$

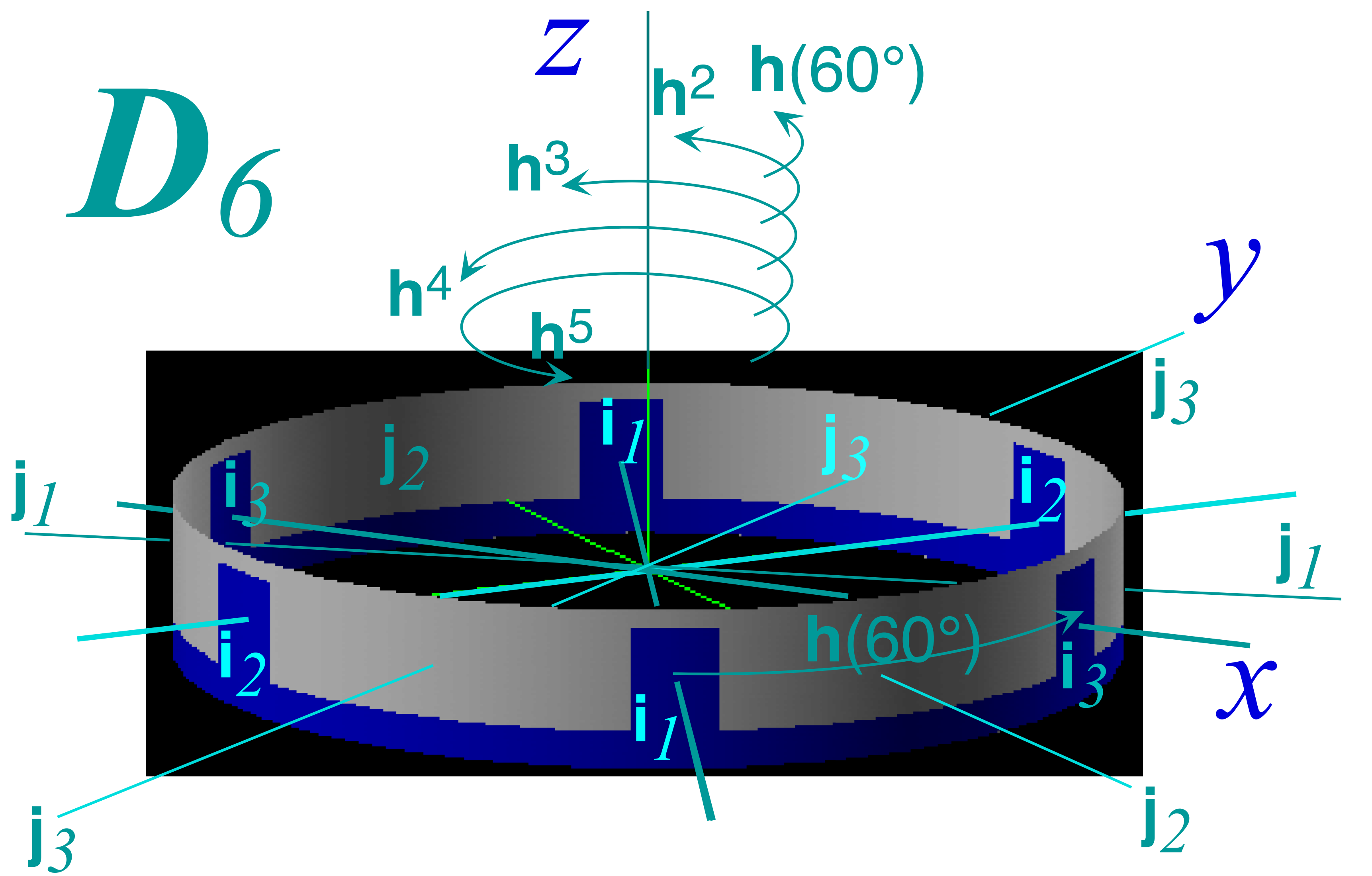
D_6 *is* product $\times$ of D_3 and C_2. Define 60° *hexagonal generator* **h** of subgroup $C_6 = \{\mathbf{1}, \mathbf{h}, \mathbf{h}^2, \mathbf{h}^3, \mathbf{h}^4\ \ \mathbf{h}^5\}$

$$D_6 = D_3 \times C_2 = \{\mathbf{1}, \mathbf{r}, \mathbf{r}^2, \mathbf{i}_1, \mathbf{i}_2, \mathbf{i}_3\} \times \{\mathbf{1}, \mathbf{R}_z\} = \{\mathbf{1}, \mathbf{r}, \mathbf{r}^2, \mathbf{i}_1, \mathbf{i}_2, \mathbf{i}_3, \mathbf{1}\cdot\mathbf{R}_z, \mathbf{r}\cdot\mathbf{R}_z, \mathbf{r}^2\cdot\mathbf{R}_z, \mathbf{i}_1\cdot\mathbf{R}_z, \mathbf{i}_2\cdot\mathbf{R}_z, \mathbf{i}_3\cdot\mathbf{R}_z\}$$

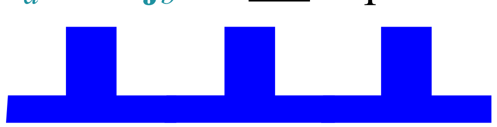
$$D_6 = D_3 \times C_2 = \qquad = \{\mathbf{1}, \mathbf{h}^2, \mathbf{h}^4, \mathbf{i}_1, \mathbf{i}_2, \mathbf{i}_3, \mathbf{h}^3, \mathbf{h}^5, \mathbf{h}, \mathbf{j}_1, \mathbf{j}_2, \mathbf{j}_3\}$$

Note: $\mathbf{h}^2 = \mathbf{r}$ and $\mathbf{h}^3 = \mathbf{R}_z$ and $\mathbf{h}^4 = \mathbf{r}^2$ and $\mathbf{h}^5 = \mathbf{r}\cdot\mathbf{R}_z$





NOTE:
The $\mathbf{i}_a$ and $\mathbf{j}_b$ do <u>not</u> flip over the potential plot.



Electrostatic potential $V(\phi)$ doesn't care which way is "up." Wells remain wells, and barriers remain barriers under all $D6$ operations.

AMOP reference links on page 2

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U(12)-Supersymmetry

Hexagonal chains: $D_{6h} \supset D_6 \supset D_3 \supset C_2$ *or* $D_{6h} \supset D_{2h} \supset D_2$ *label 6-fold bands*

Recall $C_2 \times C_2 = D_2$ characters made of two C_2 groups (*Lecture 10 p.26*)

C_2^x	$\mathbf{1}$	$\mathbf{R}_x$
+	1	1
−	1	−1

×

C_2^y	$\mathbf{1}$	$\mathbf{R}_y$
+	1	1
−	1	−1

=

$C_2^x \times C_2^y$	$\mathbf{1}\cdot\mathbf{1}$	$\mathbf{R}_x\cdot\mathbf{1}$	$\mathbf{1}\cdot\mathbf{R}_y$	$\mathbf{R}_x\cdot\mathbf{R}_y$
$+\cdot+$	$1\cdot1$	$1\cdot1$	$1\cdot1$	$1\cdot1$
$-\cdot+$	$1\cdot1$	$-1\cdot1$	$1\cdot1$	$-1\cdot1$
$+\cdot-$	$1\cdot1$	$1\cdot1$	$1\cdot(-1)$	$1\cdot(-1)$
$-\cdot-$	$1\cdot1$	$-1\cdot1$	$1\cdot(-1)$	$-1\cdot(-1)$

=

D_2	$\mathbf{1}$	$\mathbf{R}_x$	$\mathbf{R}_y$	$\mathbf{R}_z$
$++ = A_1$	1	1	1	1
$-+ = A_2$	1	-1	1	-1
$+- = B_1$	1	1	−1	−1
$-- = B_2$	1	-1	−1	1

↑ *Note common notation*

Recall $C_2 \times C_2 = D_2$ characters made of two C_2 groups (*Lecture 10 p.26*)

C_2^x	$\mathbf{1}$	$\mathbf{R}_x$
+	1	1
−	1	−1

×

C_2^y	$\mathbf{1}$	$\mathbf{R}_y$
+	1	1
−	1	−1

=

$C_2^x \times C_2^y$	$\mathbf{1}\cdot\mathbf{1}$	$\mathbf{R}_x\cdot\mathbf{1}$	$\mathbf{1}\cdot\mathbf{R}_y$	$\mathbf{R}_x\cdot\mathbf{R}_y$
$+\cdot+$	$1\cdot1$	$1\cdot1$	$1\cdot1$	$1\cdot1$
$-\cdot+$	$1\cdot1$	$-1\cdot1$	$1\cdot1$	$-1\cdot1$
$+\cdot-$	$1\cdot1$	$1\cdot1$	$1\cdot(-1)$	$1\cdot(-1)$
$-\cdot-$	$1\cdot1$	$-1\cdot1$	$1\cdot(-1)$	$-1\cdot(-1)$

=

D_2	$\mathbf{1}$	$\mathbf{R}_x$	$\mathbf{R}_y$	$\mathbf{R}_z$
$++ = A_1$	1	1	1	1
$-+ = A_2$	1	-1	1	-1
$+- = B_1$	1	1	−1	−1
$-- = B_2$	1	-1	−1	1

↑ *Note common notation*

$C_2 \times C_3 = C_6$ characters Lect.3 p36

Here made of C_2 x C_3 Cartesian product

C_2^x	$\mathbf{1}$	ρ
0_2	1	1
1_2	1	−1

×

C_3^y	$\mathbf{1}$	$\mathbf{r}^1$	$\mathbf{r}^2$
0_3	1	1	1
1_3	1	ε	ε^*
2_3	1	ε^*	ε

=

$C_2^x \times C_3^y$	$\mathbf{1}\cdot\mathbf{1}$	$\mathbf{1}\cdot\mathbf{r}^1$	$\mathbf{1}\cdot\mathbf{r}^2$	$\rho\cdot\mathbf{1}$	$\rho\cdot\mathbf{r}^1$	$\rho\cdot\mathbf{r}^2$
$0_2\cdot0_3$	$1\cdot1$	$1\cdot1$	$1\cdot1$	$1\cdot1$	$1\cdot1$	$1\cdot1$
$0_2\cdot1_3$	$1\cdot1$	$1\cdot\varepsilon$	$1\cdot\varepsilon^*$	$1\cdot1$	$1\cdot\varepsilon$	$1\cdot\varepsilon^*$
$0_2\cdot2_3$	$1\cdot1$	$1\cdot\varepsilon^*$	$1\cdot\varepsilon$	$1\cdot1$	$1\cdot\varepsilon^*$	$1\cdot\varepsilon$
$1_2\cdot0_3$	$1\cdot1$	$1\cdot1$	$1\cdot1$	$-1\cdot1$	$-1\cdot1$	$-1\cdot1$
$1_2\cdot1_3$	$1\cdot1$	$1\cdot\varepsilon$	$1\cdot\varepsilon^*$	$-1\cdot1$	$-1\cdot\varepsilon$	$-1\cdot\varepsilon^*$
$1_2\cdot2_3$	$1\cdot1$	$1\cdot\varepsilon^*$	$1\cdot\varepsilon$	$-1\cdot1$	$-1\cdot\varepsilon^*$	$-1\cdot\varepsilon$

=

C_6^{xy}	0°	120°	240°	180°	-60°	60°
0_6	$1\cdot1$	$1\cdot1$	$1\cdot1$	$1\cdot1$	$1\cdot1$	$1\cdot1$
2_6	$1\cdot1$	$1\cdot\varepsilon$	$1\cdot\varepsilon^*$	$1\cdot1$	$1\cdot\varepsilon$	$1\cdot\varepsilon^*$
4_6	$1\cdot1$	$1\cdot\varepsilon^*$	$1\cdot\varepsilon$	$1\cdot1$	$1\cdot\varepsilon^*$	$1\cdot\varepsilon$
3_6	$1\cdot1$	$1\cdot1$	$1\cdot1$	$-1\cdot1$	$-1\cdot1$	$-1\cdot1$
5_6	$1\cdot1$	$1\cdot\varepsilon$	$1\cdot\varepsilon^*$	$-1\cdot1$	$-1\cdot\varepsilon$	$-1\cdot\varepsilon^*$
1_6	$1\cdot1$	$1\cdot\varepsilon^*$	$1\cdot\varepsilon$	$-1\cdot1$	$-1\cdot\varepsilon^*$	$-1\cdot\varepsilon$

Cross product of the C_2 and D_3 characters gives all $D_6 = D_3 \times C_2$ characters.

D_3	$\mathbf{1}$	$\{\mathbf{r},\mathbf{r}^2\}$	$\{\mathbf{i}_1,\mathbf{i}_2,\mathbf{i}_3\}$
$\chi^{A_1}(\mathbf{g})$	1	1	1
$\chi^{A_2}(\mathbf{g})$	1	1	−1
$\chi^{E_1}(\mathbf{g})$	2	−1	0

×

C_2^z	$\mathbf{1}$	$\mathbf{R}_z$
(A)	1	1
(B)	1	−1

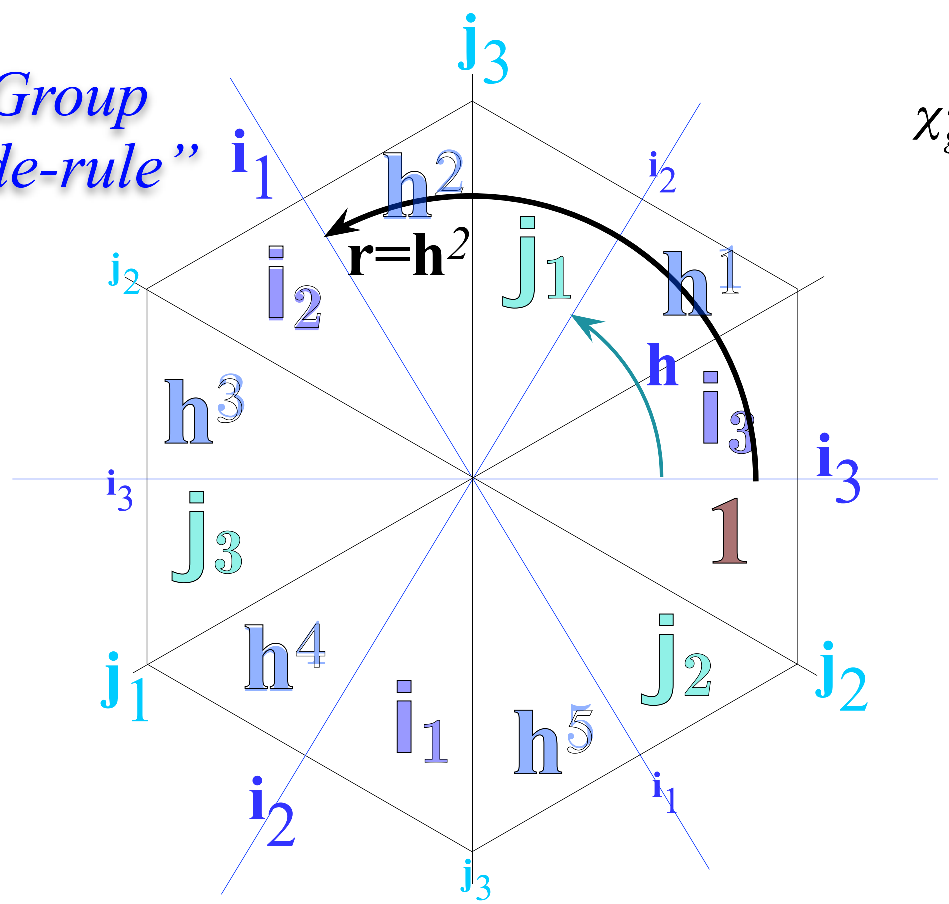
=

$D_3 \times C_2^z$	$\mathbf{1}$	$\{\mathbf{r},\mathbf{r}^2\}$	$\{\mathbf{i}_1,\mathbf{i}_2,\mathbf{i}_3\}$	$\mathbf{1}\cdot\mathbf{R}_z$	$\{\mathbf{r},\mathbf{r}^2\}\cdot\mathbf{R}_z$	$\{\mathbf{i}_1,\mathbf{i}_2,\mathbf{i}_3\}\cdot\mathbf{R}_z$
$A_1\cdot(A)$	$1\cdot 1$	$1\cdot 1$	$1\cdot 1$	$1\cdot 1$	$1\cdot 1$	$1\cdot 1$
$A_2\cdot(A)$	$1\cdot 1$	$1\cdot 1$	$-1\cdot 1$	$1\cdot 1$	$1\cdot 1$	$-1\cdot 1$
$E_2\cdot(A)$	$2\cdot 1$	$-1\cdot 1$	$0\cdot 1$	$2\cdot 1$	$-1\cdot 1$	$0\cdot 1$
$A_1\cdot(B)$	$1\cdot 1$	$1\cdot 1$	$1\cdot 1$	$1\cdot(-1)$	$1\cdot(-1)$	$1\cdot(-1)$
$A_2\cdot(B)$	$1\cdot 1$	$1\cdot 1$	$-1\cdot 1$	$1\cdot(-1)$	$1\cdot(-1)$	$-1\cdot(-1)$
$E_1\cdot(B)$	$2\cdot 1$	$-1\cdot 1$	$0\cdot 1$	$2\cdot(-1)$	$-1\cdot(-1)$	$0\cdot(-1)$

$\chi_g^{\mu}(D_6) =$

$D_3 \times C_2^z$	$\mathbf{1}$	$\{\mathbf{h}^2,\mathbf{h}^4\}$	$\{\mathbf{i}_1,\mathbf{i}_2,\mathbf{i}_3\}$	$\mathbf{h}^3$	$\{\mathbf{h},\mathbf{h}^5\}$	$\{\mathbf{j}_1,\mathbf{j}_2,\mathbf{j}_3\}$
A_1	1	1	1	1	1	1
A_2	1	1	-1	1	1	-1
E_2	2	-1	0	2	-1	0
B_2	1	1	1	-1	-1	-1
B_1	1	1	-1	-1	-1	1
E_1	2	-1	0	−2	1	0

D_6Group “slide-rule”



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or
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determines
A_p vs B_p
(+1) vs (-1)

Odd vs Even

Y-rotation
or
180° flip **j**3
determines
X_1 vs X_2
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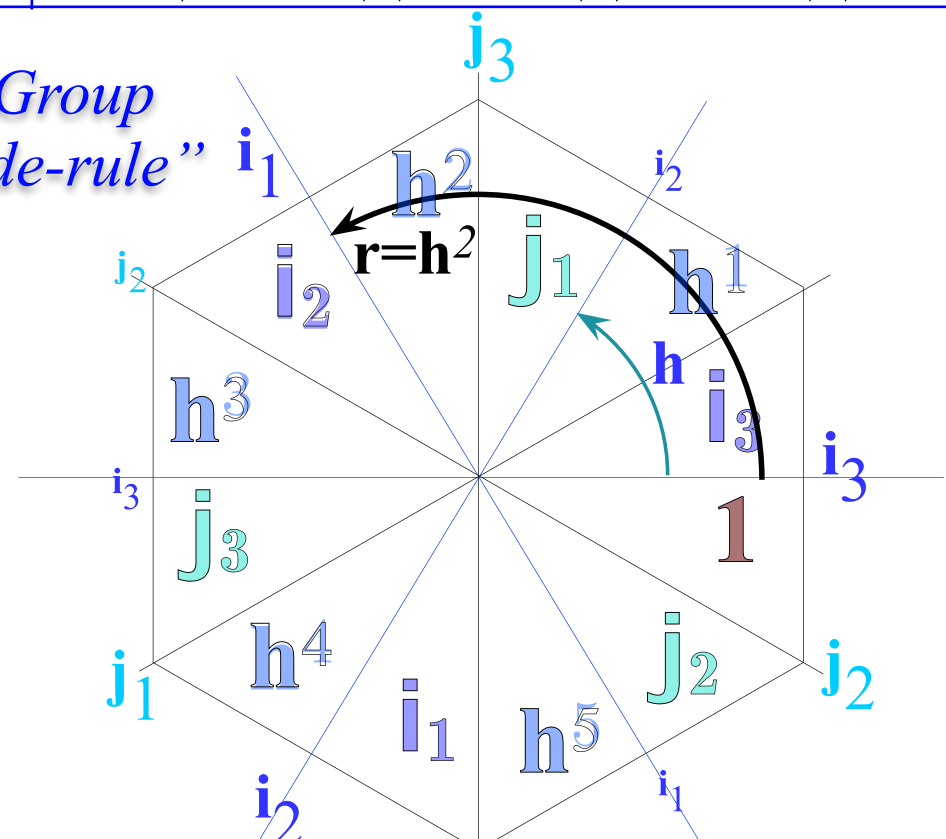
“Always-the-same vs Back-and-forth”

Recall $C_2 \times C_2 = D_2$ characters made of two C_2 groups (*Lecture 10 p.26*)

Cross product of the C_2 and D_3 characters gives all $D_6 = D_3 \times C_2$ characters.

	0°	z 120°	z -120°	180°	180°	x 180°	z 180°	z -60°	z +60°	180°	180°	y 180°
g =	**1**	**$r=h^2$**	**$r^2=h^4$**	**i_1**	**i_2**	**i_3**	**h^3**	**$h^3r=h^5$**	**$h^3r^2=h^1$**	**$h^3i_1=j_1$**	**$h^3i_2=j_2$**	**$h^3i_3=j_3$**
$D^{A_1}(g)=$	1	1	1	1	1	1	1	1	1	1	1	1
$D^{A_2}(g)=$	1	1	1	-1	-1	-1	1	1	1	-1	-1	-1
$D^{E_2}(g)=$	$\begin{pmatrix}1&0\\0&1\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{-\sqrt{3}}{2}\\\frac{\sqrt{3}}{2}&\frac{-1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{\sqrt{3}}{2}\\\frac{-\sqrt{3}}{2}&\frac{-1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{-\sqrt{3}}{2}\\\frac{-\sqrt{3}}{2}&\frac{1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{\sqrt{3}}{2}\\\frac{\sqrt{3}}{2}&\frac{1}{2}\end{pmatrix}$	$\begin{pmatrix}1&0\\0&-1\end{pmatrix}$	$\begin{pmatrix}1&0\\0&1\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{-\sqrt{3}}{2}\\\frac{\sqrt{3}}{2}&\frac{-1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{\sqrt{3}}{2}\\\frac{-\sqrt{3}}{2}&\frac{-1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{-\sqrt{3}}{2}\\\frac{-\sqrt{3}}{2}&\frac{1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{\sqrt{3}}{2}\\\frac{\sqrt{3}}{2}&\frac{1}{2}\end{pmatrix}$	$\begin{pmatrix}1&0\\0&-1\end{pmatrix}$
$D^{B_2}(g)=$	1	1	1	1	1	1	-1	-1	-1	-1	-1	-1
$D^{B_1}(g)=$	1	1	1	-1	-1	-1	-1	-1	-1	1	1	1
$D^{E_1}(g)=$	$\begin{pmatrix}1&0\\0&1\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{-\sqrt{3}}{2}\\\frac{\sqrt{3}}{2}&\frac{-1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{\sqrt{3}}{2}\\\frac{-\sqrt{3}}{2}&\frac{-1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{-\sqrt{3}}{2}\\\frac{-\sqrt{3}}{2}&\frac{1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{\sqrt{3}}{2}\\\frac{\sqrt{3}}{2}&\frac{1}{2}\end{pmatrix}$	$\begin{pmatrix}1&0\\0&-1\end{pmatrix}$	$\begin{pmatrix}-1&0\\0&-1\end{pmatrix}$	$\begin{pmatrix}\frac{1}{2}&\frac{\sqrt{3}}{2}\\\frac{-\sqrt{3}}{2}&\frac{1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{1}{2}&\frac{-\sqrt{3}}{2}\\\frac{\sqrt{3}}{2}&\frac{1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{1}{2}&\frac{\sqrt{3}}{2}\\\frac{\sqrt{3}}{2}&\frac{-1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{1}{2}&\frac{-\sqrt{3}}{2}\\\frac{-\sqrt{3}}{2}&\frac{-1}{2}\end{pmatrix}$	$\begin{pmatrix}-1&0\\0&1\end{pmatrix}$

D_6Group "slide-rule"



Unit translation or 60° *hex rotation* **h** *determines* *A_p vs B_p* (+1) vs (-1)

Y-rotation or 180° *flip* **j_3** *determines* *X_1 vs X_2* (+1) vs (-1)

"Always-the-same vs Back-and-forth"

Odd vs Even

Cross product of the C_2 and D_3 characters gives all $D_6 = D_3 \times C_2$ characters.

	0°	z 120°	z -120°	180°	180°	x 180°	z 180°	z -60°	z +60°	180°	180°	y 180°
g =	**1**	$\mathbf{r=h^2}$	$\mathbf{r^2=h^4}$	$\mathbf{i_1}$	$\mathbf{i_2}$	$\mathbf{i_3}$	$\mathbf{h^3}$	$\mathbf{h^3r=h^5}$	$\mathbf{h^3r^2=h^1}$	$\mathbf{h^3i_1=j_1}$	$\mathbf{h^3i_2=j_2}$	$\mathbf{h^3i_3=j_3}$
$D^{A_1}(g)=$	1	1	1	1	1	1	1	1	1	1	1	1
$D^{A_2}(g)=$	1	1	1	-1	-1	-1	1	1	1	-1	-1	-1
$D^{E_2}(g)=$	$\begin{pmatrix}1&0\\0&1\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{-\sqrt{3}}{2}\\\frac{\sqrt{3}}{2}&\frac{-1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{\sqrt{3}}{2}\\\frac{-\sqrt{3}}{2}&\frac{-1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{-\sqrt{3}}{2}\\\frac{-\sqrt{3}}{2}&\frac{1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{\sqrt{3}}{2}\\\frac{\sqrt{3}}{2}&\frac{1}{2}\end{pmatrix}$	$\begin{pmatrix}1&0\\0&-1\end{pmatrix}$	$\begin{pmatrix}1&0\\0&1\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{-\sqrt{3}}{2}\\\frac{\sqrt{3}}{2}&\frac{-1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{\sqrt{3}}{2}\\\frac{-\sqrt{3}}{2}&\frac{-1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{-\sqrt{3}}{2}\\\frac{-\sqrt{3}}{2}&\frac{1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{\sqrt{3}}{2}\\\frac{\sqrt{3}}{2}&\frac{1}{2}\end{pmatrix}$	$\begin{pmatrix}1&0\\0&-1\end{pmatrix}$
$D^{B_2}(g)=$	1	1	1	1	1	1	-1	-1	-1	- 1	-1	-1
$D^{B_1}(g)=$	1	1	1	-1	-1	-1	-1	-1	-1	1	1	1
$D^{E_1}(g)=$	$\begin{pmatrix}1&0\\0&1\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{-\sqrt{3}}{2}\\\frac{\sqrt{3}}{2}&\frac{-1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{\sqrt{3}}{2}\\\frac{-\sqrt{3}}{2}&\frac{-1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{-\sqrt{3}}{2}\\\frac{-\sqrt{3}}{2}&\frac{1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{\sqrt{3}}{2}\\\frac{\sqrt{3}}{2}&\frac{1}{2}\end{pmatrix}$	$\begin{pmatrix}1&0\\0&-1\end{pmatrix}$	$\begin{pmatrix}-1&0\\0&-1\end{pmatrix}$	$\begin{pmatrix}\frac{1}{2}&\frac{\sqrt{3}}{2}\\\frac{-\sqrt{3}}{2}&\frac{1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{1}{2}&\frac{-\sqrt{3}}{2}\\\frac{\sqrt{3}}{2}&\frac{1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{1}{2}&\frac{\sqrt{3}}{2}\\\frac{\sqrt{3}}{2}&\frac{-1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{1}{2}&\frac{-\sqrt{3}}{2}\\\frac{-\sqrt{3}}{2}&\frac{-1}{2}\end{pmatrix}$	$\begin{pmatrix}-1&0\\0&1\end{pmatrix}$

Unit translation
or
60° *hex rotation* **h**
determines
A_p vs B_p
(+1) vs (-1)

Y-rotation
or
180° *flip* $\mathbf{j}_3$
determines
X_1 vs X_2
(+1) vs (-1)

$D_6 \supset C_2(j_3)$	0_2	1_2
A_1	1	·
A_2	·	1
E_2	1	1
B_2	·	1
B_1	1	·
E_1	1	1

$D_6 \supset C_6(h)$	0_6	1_6	2_6	3_6	4_6	5_6
A_1	1	·	·	·	·	·
A_2	1	·	·	·	·	·
E_2	·	·	1	·	1	·
B_2	·	·	·	1	·	·
B_1	·	·	·	1	·	·
E_1	·	1	·	·	·	1

AMOP reference links on page 2

2.26.18 class 14.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

Discrete symmetry subgroups of O(3) using Mock-Mach principle: $D_3 \sim C_{3v}$ LAB vs BOD
Vibrational eigensolutions, $D_6 \sim C_{6v}$ bands, subgroup correlation, and Frobenius reciprocity

Review: *H-matrix Global vs Local symmetry*

Molecular vibration K-matrix symmetry analogous to quantum H-matrix

Molecular K-matrix construction

$D_3 \supset C_2(i_3)$ local-symmetry K-matrix eigensolutions

D_3-direct-connection K-matrix eigenstates mix local symmetry

$D_3 \supset C_3(\mathbf{r}^{\pm 1})$ moving-wave local symmetry K-matrix "Coriolis" eigensolutions

Applied symmetry reduction and splitting

Subduced irep $D^\alpha(D^3) \downarrow C_2 = d^{0_2} \oplus d^{1_2} \oplus ..$ correlation

Subduced irep $D^\alpha(D^3) \downarrow C_3 = d^{0_3} \oplus d^{1_3} \oplus ..$ correlation

Spontaneous symmetry breaking and clustering: Frobenius Reciprocity and band structure

Induced rep $d^a(C_2) \uparrow D^3 = D^\alpha \oplus D^\beta \oplus ..$ correlation

Induced rep $d^a(C_3) \uparrow D^3 = D^\alpha \oplus D^\beta \oplus ..$ correlation

D_6 symmetry and Hexagonal Bands

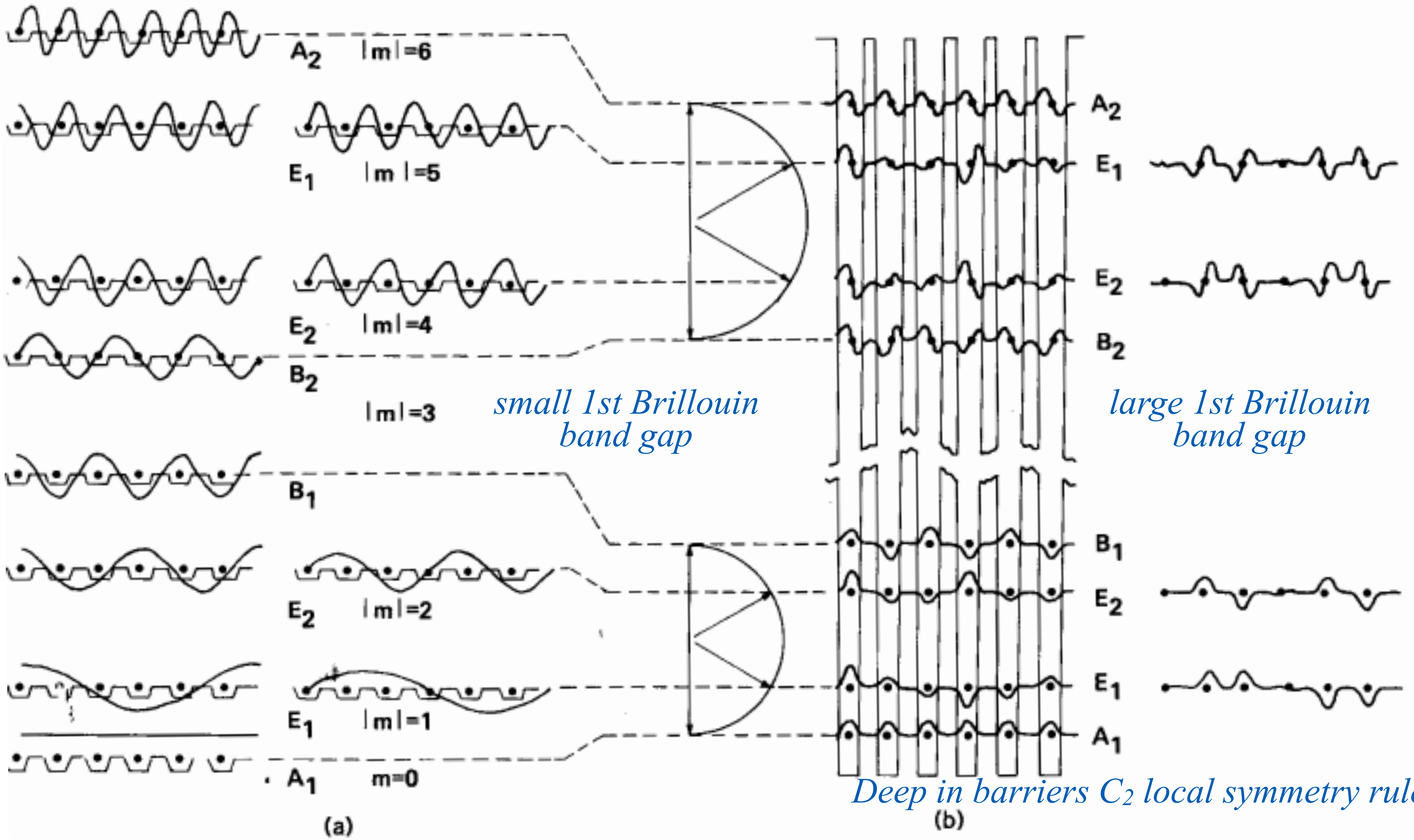
Cross product of the C_2 and D_3 characters gives all $D_6 = D_3 \times C_2$ characters and ireps

D_6 Band structure and related Global vs Local induced representations, *D_4 example*

U(12)-Supersymmetry

D_6 Band structure and related Global vs Local induced representations

High above low barriers $D_6 \supset C_6$ global symmetry rules



Deep in barriers C_2 local symmetry rules

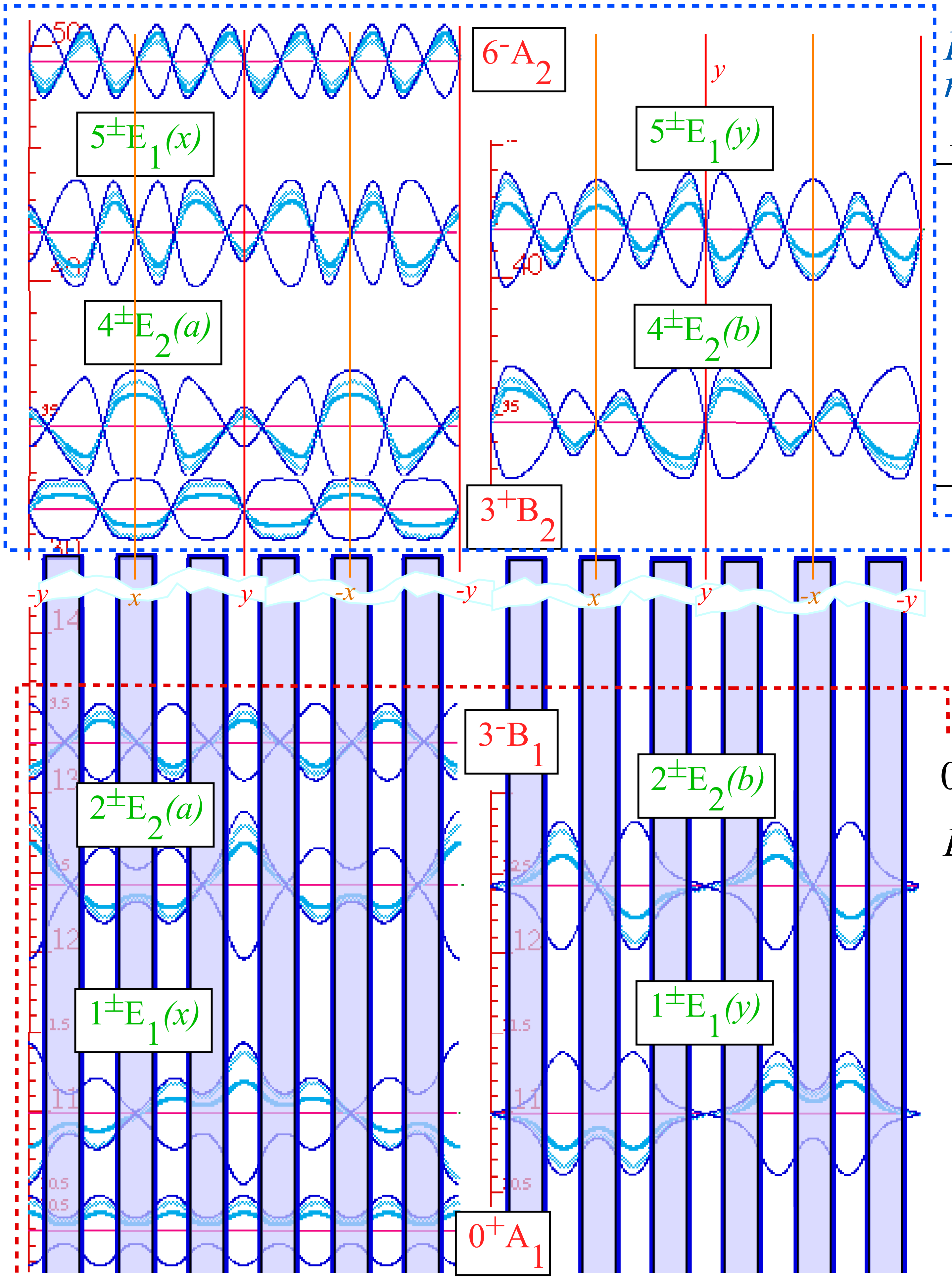
Figure 3.6.5 One-dimensional Bohr and Bloch waves in D_6 symmetry. (a) Weak D_6 potential. (b) Strong D_6 potential.

PSDS Ch.3 p 50.

D_6
Band structure and related Global vs Local induced representations

(BohrIt Mac OS-9)

D_6
Band structure
QTCA Unit 5 p96



Low barrier->D_6 global symm.
m_6 still valid quantum number

$D_6 \supset C_6(h)$	0_6	1_6	2_6	3_6	4_6	5_6
A_1	1	·	·	·	·	·
A_2	1	·	·	·	·	·
E_2	·	·	1	·	1	·
B_2	·	·	·	1	·	·
B_1	·	·	·	1	·	·
E_1	·	1	·	·	·	1

$1_2 \uparrow D_6 \sim A_2 \oplus E_2 \oplus E_1 \oplus B_2$

Odd Band or Cluster

$0_2 \uparrow D_6 \sim A_1 \oplus E_1 \oplus E_2 \oplus B_1$

Even Band or Cluster

$D_6 \supset C_2(j_3)$	0_2	1_2
A_1	1	·
A_2	·	1
E_2	1	1
B_2	·	1
B_1	1	·
E_1	1	1

AMOP reference links on page 2

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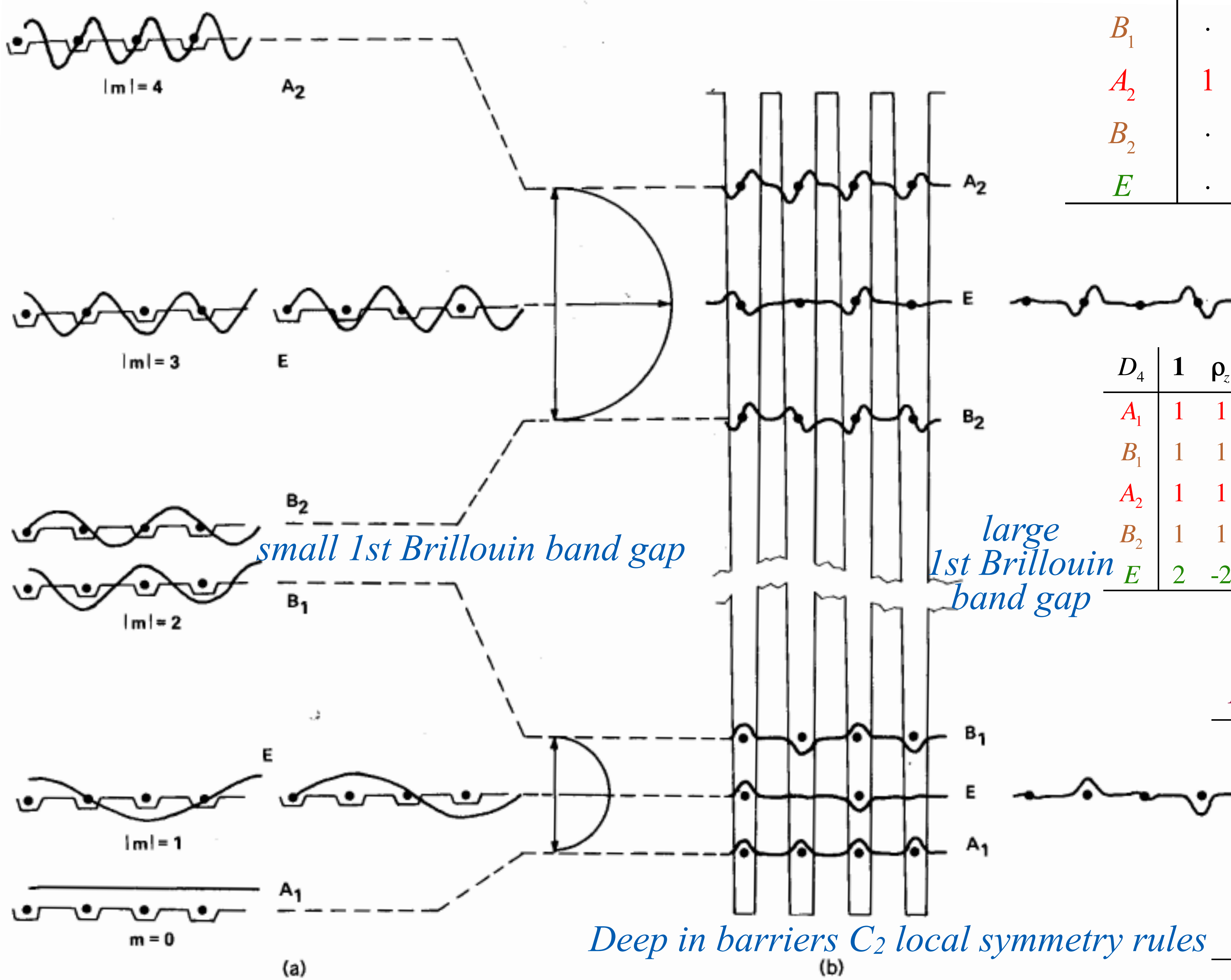
D_6 Band structure and related Global vs Local induced representations, ➡ *D_4 example*

U(12)-Supersymmetry

D_4 :Simplest example of ring-lattice band structure and symmetry

$D_4 \downarrow C_4$	0_4	1_4	2_4	-1_4
A_1	1	·	·	·
B_1	·	·	1	·
A_2	1	·	·	·
B_2	·	·	1	·
E	·	1	·	1

High above low barriers $D_4 \supset C_4$ global symmetry rules



small 1st Brillouin band gap

large 1st Brillouin band gap

Deep in barriers C_2 local symmetry rules

D_4	**1**	ρ_z	$\mathbf{R}_z$	$\rho_{x,y}$	$\mathbf{i}_{3,4}$
A_1	1	1	1	1	1
B_1	1	1	-1	1	-1
A_2	1	1	1	-1	-1
B_2	1	1	-1	-1	1
E	2	-2	0	0	0

$D_4 \downarrow C_2$	0_2	1_2
A_1	1	·
B_1	·	1
A_2	1	·
B_2	·	1
E	1	1

Figure 3.6.2 One-dimensional Bohr and Bloch waves in D_4 symmetry. (a) Weak D_4 potential. (b) Strong D_4 potential.

D_4 Mol-vibe band-analog animation ?

PSDS Ch.3 p 45.

AMOP reference links on page 2

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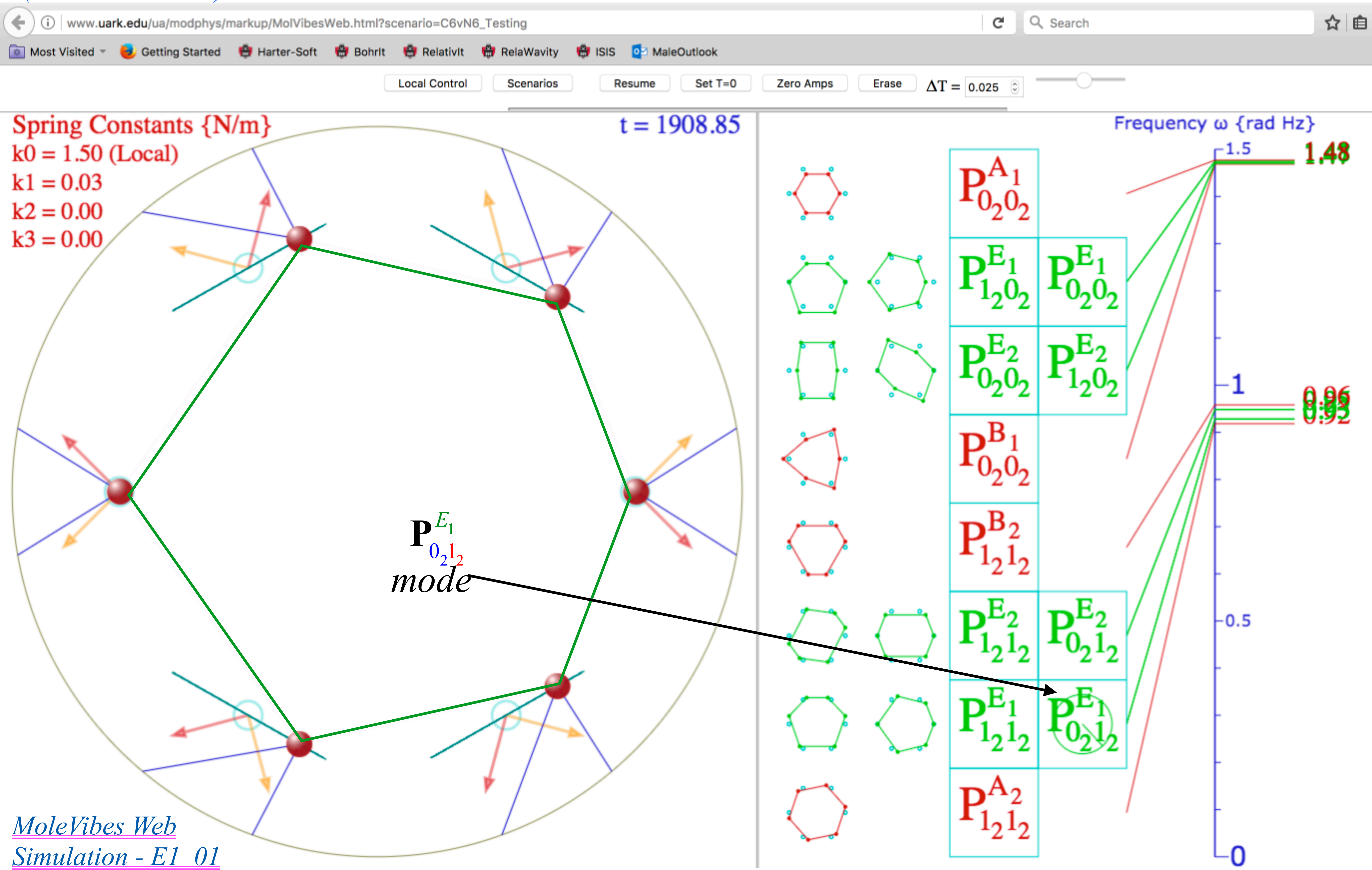
➡ *D_6 Band structure and related Global vs Local induced representations,* *D_4 example*

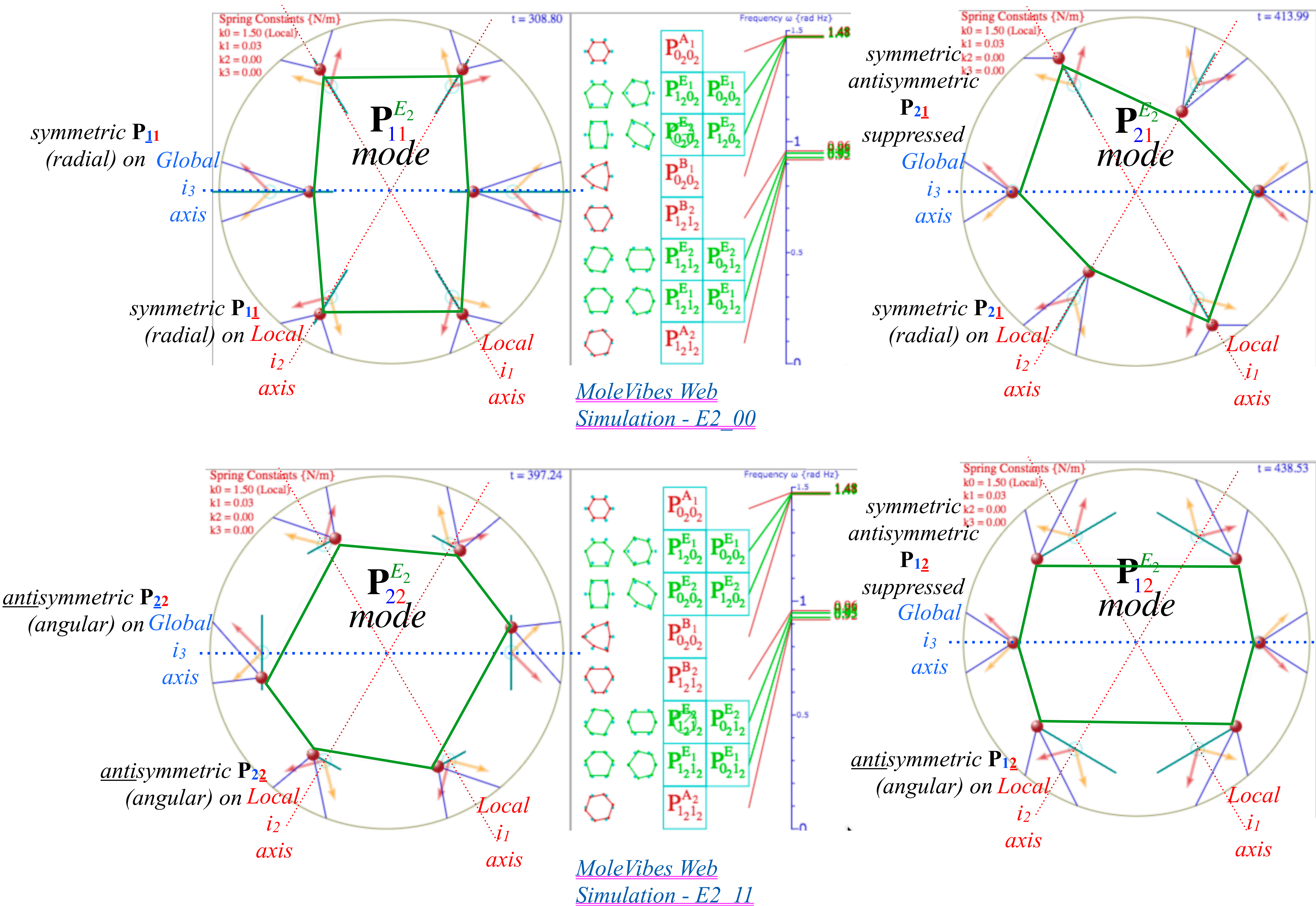
U(12)-Supersymmetry

D_6 Band structure and related induced representations (Web MolVibes)

The testing config:
http://www.uark.edu/ua/modphys/markup/MolVibesWeb.html?scenario=C6vN6_Testing



MoleVibes Web Simulation - E1_01



Spring Constants {N/m}
k0 = 1.50 (Local)
k1 = 0.03
k2 = 0.00
k3 = 0.00
t = 308.80
P E2 11 mode
symmetric P11 (radial) on Global i3 axis
symmetric P11 (radial) on Local i2 axis
Local i1 axis
Frequency ω (rad Hz)
1.48
0.96
0.95
MoleVibes Web Simulation - E2_00
t = 413.99
symmetric antisymmetric P21 suppressed Global i3 axis
P E2 21 mode
symmetric P21 (radial) on Local i2 axis
Local i1 axis
t = 397.24
P E2 22 mode
antisymmetric P22 (angular) on Global i3 axis
antisymmetric P22 (angular) on Local i2 axis
Local i1 axis
MoleVibes Web Simulation - E2_11
t = 438.53
symmetric antisymmetric P12 suppressed Global i3 axis
P E2 12 mode
antisymmetric P12 (angular) on Local i2 axis
Local i1 axis

AMOP reference links on page 2

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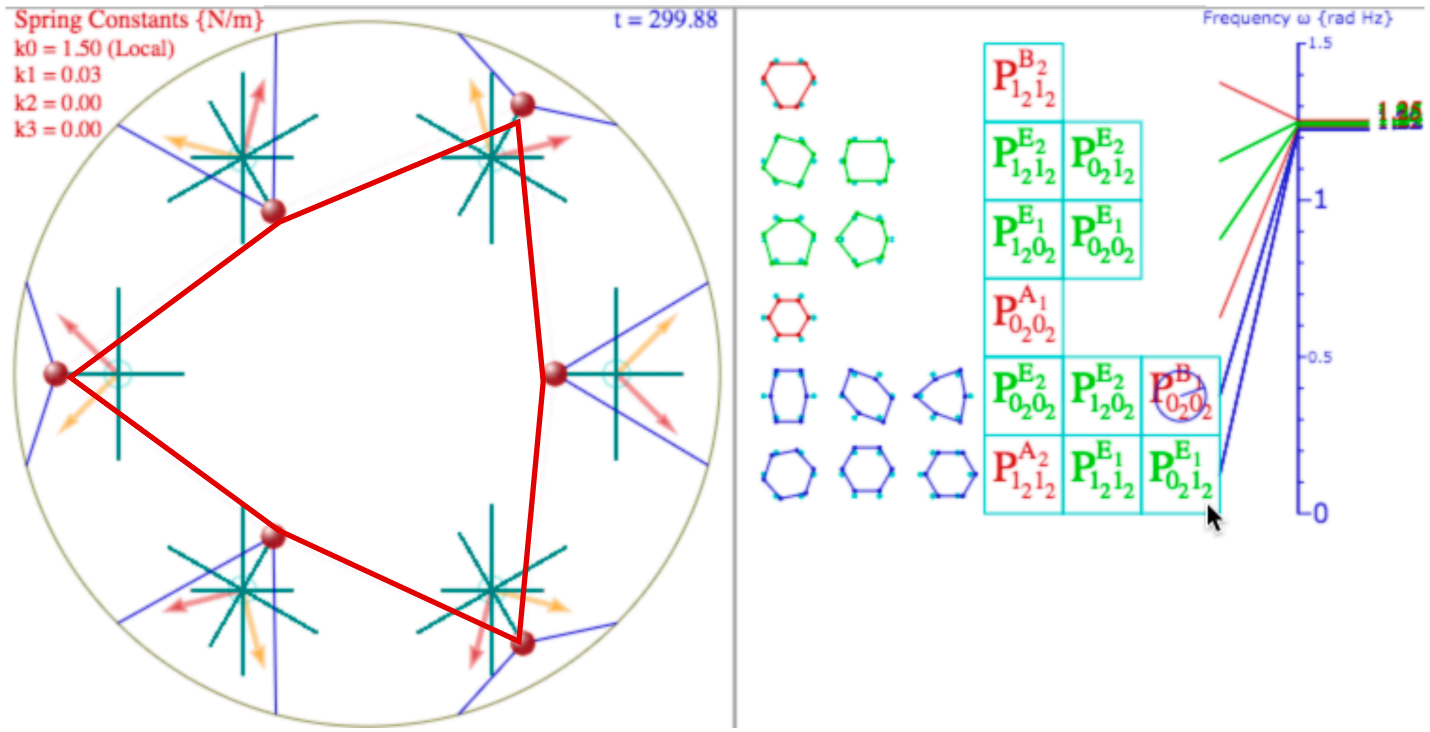
D_6 Band structure and related Global vs Local induced representations, *D_4 example*

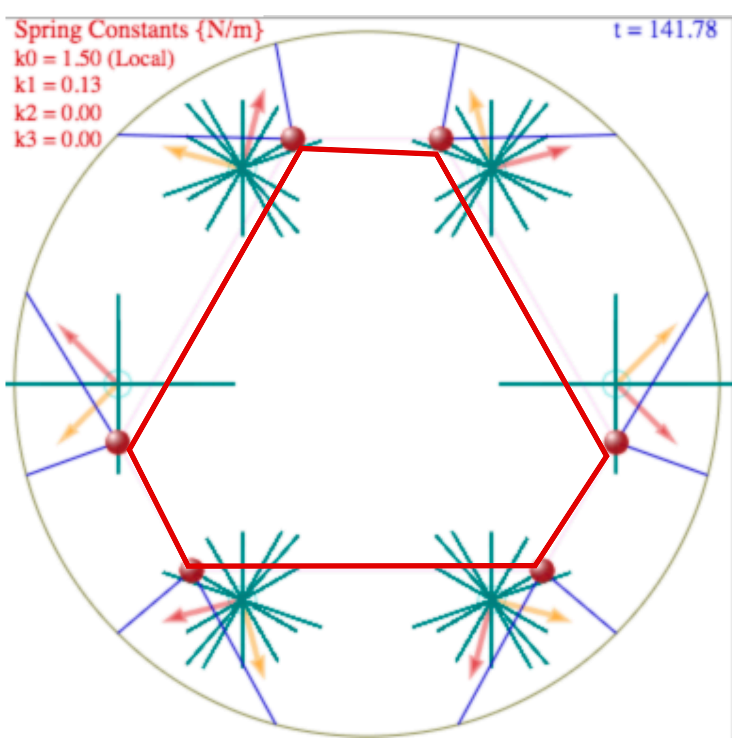
→ *U(12)-Supersymmetry*

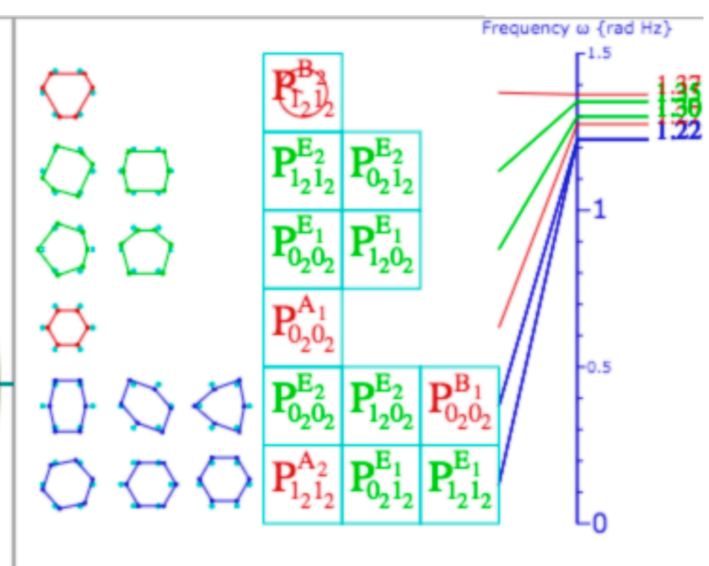
U(12)-Supersymmetry: When D_6 Band structure approaches single 12-fold degeneracy
Setting mutually orthogonal external k_0 connection springs (and tiny k_1, k_2,.. coupling)



U(12)-Supersymmetry
QTCA Unit5 p89

Even moderate k_1 coupling lifts a band of single-doublet-doublet-singlet above 6-fold degenerate sextet





Local symmetry-asymmetry is well broken
as strictly radial or angular paths are avoided by masses off x-axis

D_6 Band structure and related induced representations (Mac OS-9)